Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssspta1621con

PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

| | | |
|---|---|---|
| NEWS 1 | | Web Page for STN Seminar Schedule - N. America |
| NEWS 2 | JAN 02 | STN pricing information for 2008 now available |
| NEWS 3 | JAN 16 | CAS patent coverage enhanced to include exemplified prophetic substances |
| NEWS 4 | JAN 28 | USPATFULL, USPAT2, and USPATOLD enhanced with new custom IPC display formats |
| NEWS 5 | JAN 28 | MARPAT searching enhanced |
| NEWS 6 | JAN 28 | USGENE now provides USPTO sequence data within 3 days of publication |
| NEWS 7 | JAN 28 | TOXCENTER enhanced with reloaded MEDLINE segment |
| NEWS 8 | JAN 28 | MEDLINE and LMEDLINE reloaded with enhancements |
| NEWS 9 | FEB 08 | STN Express, Version 8.3, now available |
| NEWS 10 | FEB 20 | PCI now available as a replacement to DPCI |
| NEWS 11 | FEB 25 | IFIREF reloaded with enhancements |
| NEWS 12 | FEB 25 | IMSPRODUCT reloaded with enhancements |
| NEWS 13 | FEB 29 | WPINDEX/WPIDS/WPIX enhanced with ECLA and current U.S. National Patent Classification |
| NEWS 14 | MAR 31 | IFICDB, IFIPAT, and IFIUDB enhanced with new custom IPC display formats |
| NEWS 15 | MAR 31 | CAS REGISTRY enhanced with additional experimental spectra |
| NEWS 16 | MAR 31 | CA/CAplus and CASREACT patent number format for U.S. applications updated |
| NEWS 17 | MAR 31 | LPCI now available as a replacement to LDPCI |
| NEWS 18 | MAR 31 | EMBASE, EMBAL, and LEMBASE reloaded with enhancements |
| NEWS 19 | APR 04 | STN AnaVist, Version 1, to be discontinued |
| NEWS 20 | APR 15 | WPIDS, WPINDEX, and WPIX enhanced with new predefined hit display formats |
| NEWS 21 | APR 28 | EMBASE Controlled Term thesaurus enhanced |
| NEWS 22 | APR 28 | IMSRESEARCH reloaded with enhancements |
| NEWS 23 | MAY 30 | INPAFAMDB now available on STN for patent family searching |
| NEWS 24 | MAY 30 | DGENE, PCTGEN, and USGENE enhanced with new homology sequence search option |
| NEWS 25 | JUN 06 | EPFULL enhanced with 260,000 English abstracts |
| NEWS 26 | JUN 06 | KOREAPAT updated with 41,000 documents |
| NEWS 27 | JUN 13 | USPATFULL and USPAT2 updated with 11-character patent numbers for U.S. applications |
| NEWS 28 | JUN 19 | CAS REGISTRY includes selected substances from web-based collections |
| NEWS 29 | JUN 25 | CA/CAplus and USPAT databases updated with IPC reclassification data |

NEWS 30 JUN 30 AEROSPACE enhanced with more than 1 million U.S. patent records
NEWS 31 JUN 30 EMBASE, EMBAL, and LEMBASE updated with additional options to display authors and affiliated organizations
NEWS 32 JUN 30 STN on the Web enhanced with new STN AnaVist Assistant and BLAST plug-in
NEWS 33 JUN 30 STN AnaVist enhanced with database content from EPFULL

NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3,
AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.

NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS LOGIN Welcome Banner and News Items
NEWS IPC8 For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 10:01:41 ON 16 JUL 2008

=> file casreact

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| FULL ESTIMATED COST | 0.21 | 0.21 |

FILE 'CASREACT' ENTERED AT 10:02:07 ON 16 JUL 2008
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT


FILE CONTENT:1840 - 12 Jul 2008 VOL 149 ISS 3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

**********
* *
* CASREACT now has more than 13.8 million reactions *
* *
**********

Some CASREACT records are derived from the ZIC/VINITI database (1974-1999) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance

identification.

=>
Uploading C:\Program Files\Stnexp\Queries\dd4.str

chain nodes :
1 2
chain bonds :
1-2
exact/norm bonds :
1-2

Match level :
1:Atom 2:CLASS
Generic attributes :
1:
Saturation : Unsaturated

fragments assigned product role:
containing 1
reaction site bonds:
1-2:CC

L1 STRUCTURE UPLOADED

=> s l1
SAMPLE SEARCH INITIATED 10:02:27 FILE 'CASREACT'
SCREENING
SCREENING COMPLETE - 766258 REACTIONS TO VERIFY FROM 33516 DOCUMENTS

0.7% DONE 5000 VERIFIED 1275 HIT RXNS 50 DOCS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.18

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**
PROJECTED VERIFICATIONS: 15304789 TO 15304787
PROJECTED ANSWERS: 605483 TO 611879

L2 50 SEA SSS SAM L1 ( 1275 REACTIONS)

=>
Uploading C:\Program Files\Stnexp\Queries\dd5.str

chain nodes :
1 2 4
chain bonds :
1-2
exact/norm bonds :
1-2

G1:Co,Ni,Pt,Rh,Ru

Match level :
1:Atom 2:CLASS 4:CLASS
Generic attributes :
1:
Saturation : Unsaturated

fragments assigned product role:
containing 1
reaction site bonds:
1-2:CC

L3 STRUCTURE UPLOADED

=> s l3
SAMPLE SEARCH INITIATED 10:05:19 FILE 'CASREACT'
SCREENING COMPLETE - 24836 REACTIONS TO VERIFY FROM 2088 DOCUMENTS

20.1% DONE 5000 VERIFIED 623 HIT RXNS 50 DOCS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.02

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED VERIFICATIONS: 487420 TO 506020
PROJECTED ANSWERS: 17474 TO 21148

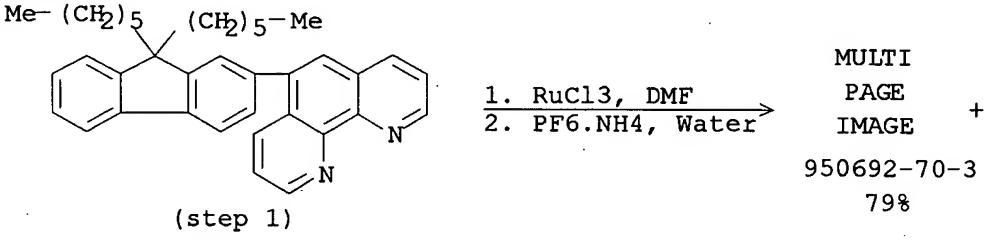
L4 50 SEA SSS SAM L3 ( 623 REACTIONS)

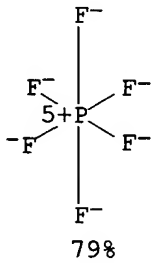
=> d scan

L4 50 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI Novel ruthenium(II) and zinc(II) complexes for two-photon absorption related applications

RX(4) OF 17



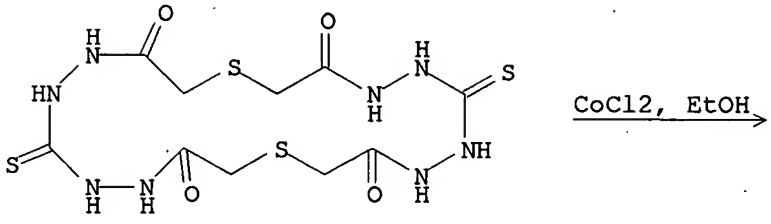




HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

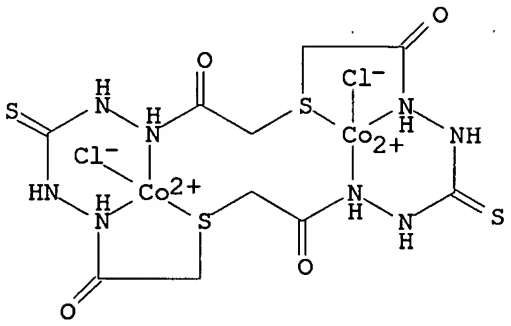
L4 50 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI The Spectroscopy: A modern technology in the characterization of novel macrocyclic ligand and its homo-bi-nuclear cobalt (II) complexes

RX(1) OF 9




RX(1) OF 9



2 Cl⁻
57%

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L4 50 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI Imidazole-based nickel(II) and cobalt(II) coordination complexes for potential use as models for histidine containing metalloproteins

RX(1) OF 6 - REACTION DIAGRAM NOT AVAILABLE

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L4 50 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI FTIR, magnetic, mass spectral, XRD and thermal studies of metal chelates of tenoxicam

RX(3) OF 6 - REACTION DIAGRAM NOT AVAILABLE

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L4 50 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI Synthesis and characterization of new metal-free and metallophthalocyanines containing macrobicyclic moieties

RX(9) OF 25 - REACTION DIAGRAM NOT AVAILABLE

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L4 50 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI Synthesis of bimetallic ruthenium complexes with an azobenzene-containing ligand

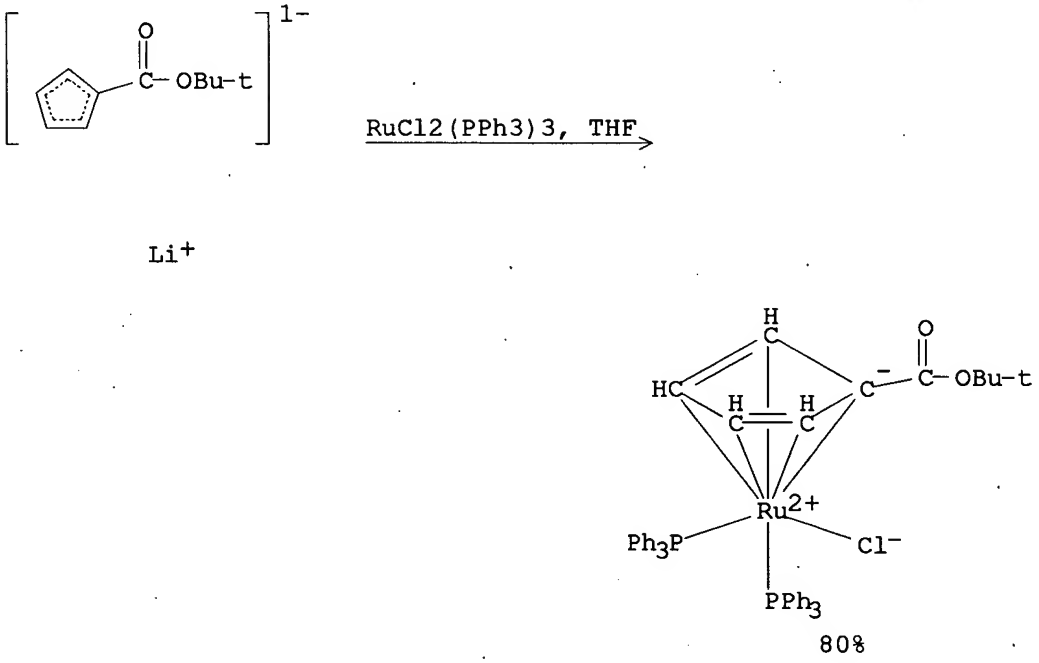
RX(1) OF 3 - REACTION DIAGRAM NOT AVAILABLE

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L4 50 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI Synthesis and properties of carboxy-substituted half-sandwich ruthenium complexes with chelating bisphosphine ligands (η5-C5H4CO2H)Ru(η2-L)X (X = I, H)

RX(2) OF 47



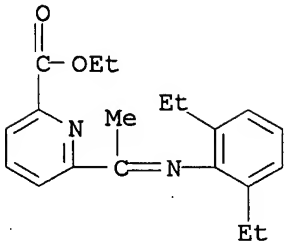

80%

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):end

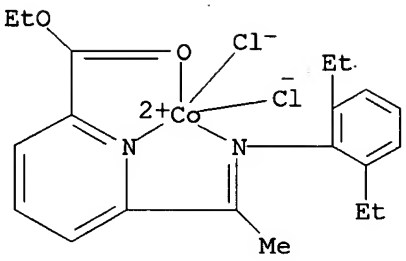
=> d l4 crd 10

L4 ANSWER 10 OF 50 CASREACT COPYRIGHT 2008 ACS on STN

RX(4) OF 10



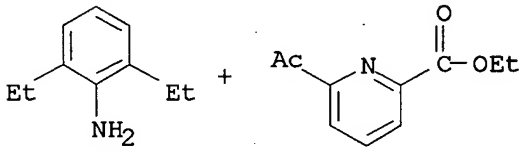
CoCl2, EtOH, Et2O



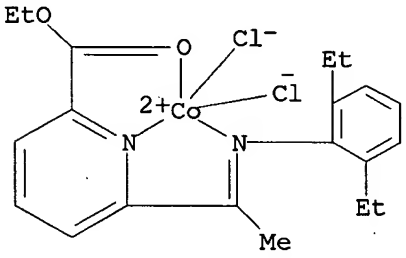
65%

CON: 7 days, room temperature

RX(7) OF 10 - 2 STEPS



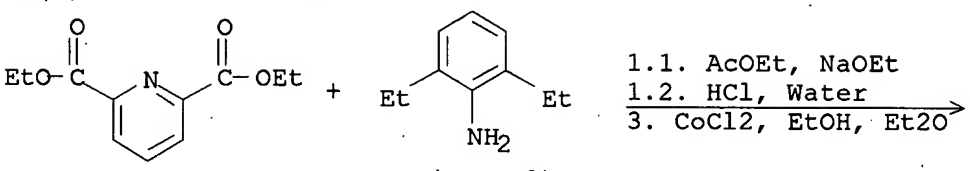
2. CoCl2, EtOH, Et2O



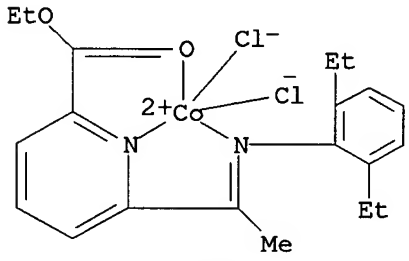
65%

NOTE: 1) microwave irradn., 800W used
CON: STEP(1) 35 minutes
STEP(2) 7 days, room temperature

RX(9) OF 10 - 3 STEPS



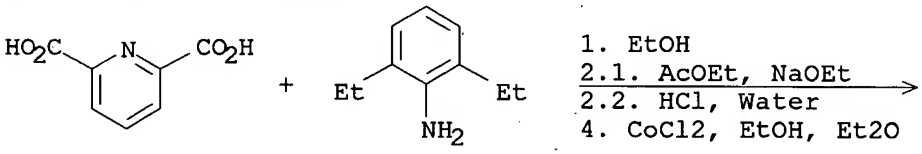

(step 2)



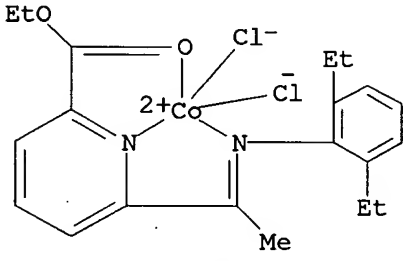

65%

NOTE: 2) microwave irradn., 800W used
CON: STEP(1.1) 12 hours, reflux; overnight, room temperature
STEP(1.2) 7 - 8 hours, reflux
STEP(2) 35 minutes
STEP(3) 7 days, room temperature

RX(10) OF 10 - 4 STEPS




(step 3)




65%

NOTE: 1) no exptl. detail, 3) microwave irradn., 800W used
CON: STEP(2.1) 12 hours, reflux; overnight, room temperature
STEP(2.2) 7 - 8 hours, reflux
STEP(3) 35 minutes
STEP(4) 7 days, room temperature

=> d his

```
     (FILE 'HOME' ENTERED AT 10:01:41 ON 16 JUL 2008)

     FILE 'CASREACT' ENTERED AT 10:02:07 ON 16 JUL 2008
L1                STRUCTURE UPLOADED
L2             50 S L1
L3                STRUCTURE UPLOADED
L4             50 S L3

=> s l4 and ?deuterat?
           3715 ?DEUTERAT?
L5            0 L4 AND ?DEUTERAT?

=> d his

     (FILE 'HOME' ENTERED AT 10:01:41 ON 16 JUL 2008)

     FILE 'CASREACT' ENTERED AT 10:02:07 ON 16 JUL 2008
L1                STRUCTURE UPLOADED
L2             50 S L1
L3                STRUCTURE UPLOADED
L4             50 S L3
L5              0 S L4 AND ?DEUTERAT?

=> s l3 ful
FULL SEARCH INITIATED 10:08:22 FILE 'CASREACT'
SCREENING COMPLETE -   528033 REACTIONS TO VERIFY FROM    41993 DOCUMENTS

 95.4% DONE  503873 VERIFIED  180280 HIT RXNS (    34 INCOMP)   16646 DOCS

100.0% DONE  528033 VERIFIED  188945 HIT RXNS (    34 INCOMP)   17407 DOCS
SEARCH TIME: 00.00.25

L6         17407 SEA SSS FUL L3 (188945 REACTIONS)

=> s l6/com
L7        16789 L6/COM

=> s l7 and ?deuterat?
           3715 ?DEUTERAT?
L8          103 L7 AND ?DEUTERAT?

=> D IBIB ABS HITIND CRD 1
'HITIND' IS NOT A VALID FORMAT FOR FILE 'CASREACT'

The following are valid formats:

ABS -------- GI and AB
ALL -------- BIB, AB, IND, RE, Single-step Reactions
APPS ------- AI, PRAI
BIB -------- AN, plus Bibliographic Data
CAN -------- List of CA abstract numbers without answer numbers
CBIB ------- AN, plus Compressed Bibliographic Data
DALL ------- ALL, delimited (end of each field identified)
IABS ------- ABS, indented with text labels
IALL ------- ALL, indented with text labels
IBIB ------- BIB, indented with text labels
IND -------- Indexing data
```

IPC -------- International Patent Classifications
ISTD ------- STD, indented with text labels
OBIB -------- AN, plus Bibliographic Data (original)
OIBIB ------- OBIB, indented with text labels

SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

MAX -------- Same as ALL
PATS ------- PI, SO
SCAN ------- TI and FCRD (random display, no answer number. SCAN must be entered on the same line as DISPLAY, e.g., D SCAN.)
SSRX ------- Single-Step Reactions (Map, Diagram, and Summary for all single-step reactions)
STD -------- BIB, IPC, and NCL

CRD -------- Compact Display of All Hit Reactions
CRDREF ----- Compact Reaction Display and SO, PY for Reference
FHIT ------- Reaction Map, Diagram, and Summary for first hit reaction
FHITCBIB --- FHIT, AN plus CBIB
FCRD ------- First hit in Compact Reaction Display (CRD) format
FCRDREF ---- First hit in Compact Reaction Display (CRD) format with CA reference information (SO, PY). (Default)
FPATH ------ PATH, plus Reaction Summary for the "long path"
FSPATH ----- SPATH, plus Reaction Summary for the "short path"
HIT -------- Reaction Map, Reaction Diagram, and Reaction Summary for all hit reactions and fields containing hit terms
OCC -------- All hit fields and the number of occurrences of the hit terms in each field. Includes total number of HIT, PATH, SPATH reactions. Labels reactions that have incomplete verifications.
PATH ------- Reaction Map and Reaction Diagram for the "long path". Displays all hit reactions, except those whose steps are totally included within another hit reaction which is displayed
RX --------- Hit Reactions (Map, Diagram, Summary for all hit reactions)
RXG -------- Hit Reaction Graphics (Map and Diagram for all hit reactions)
RXL -------- Hit Reaction Long (Map, Diagram, Summary for all hit reactions)
RXS -------- Hit Reaction Summariers (Map and Summary for all hit reactions)
SPATH ------ Reaction Map and Reaction Diagram for the "short path". Displays all single step reactions which contain a hit substance. Also displays those multistep reactions that have a hit substance in both the first and last steps of the reaction, except for those hit reactions whose steps are totally included within another hit reaction which is displayed

To display a particular field or fields, enter the display field codes. For a list of the display field codes, enter HELP DFIELDS at an arrow prompt (=>). Examples of combinations include: D TI; D BIB RX; D TI, AU, FCRD. The information is displayed in the same order as the specification. All of the formats, except CRD, CRDREF, FHIT, PATH, FPATH, SPATH, FSPATH, FCRD, FCRDREF, HIT, RX, RXG, RXS, SCAN, and OCC, may be used with the DISPLAY command to display the record for a specified Accession Number.

ENTER DISPLAY FORMAT (FCRDREF):D IBIB ABS CRD 1
'D' IS NOT A VALID FORMAT FOR FILE 'CASREACT'

The following are valid formats:

ABS -------- GI and AB
ALL -------- BIB, AB, IND, RE, Single-step Reactions
APPS ------- AI, PRAI
BIB -------- AN, plus Bibliographic Data
CAN -------- List of CA abstract numbers without answer numbers
CBIB ------- AN, plus Compressed Bibliographic Data
DALL ------- ALL, delimited (end of each field identified)
IABS ------- ABS, indented with text labels
IALL ------- ALL, indented with text labels
IBIB ------- BIB, indented with text labels
IND -------- Indexing data
IPC -------- International Patent Classifications
ISTD ------- STD, indented with text labels
OBIB -------- AN, plus Bibliographic Data (original)
OIBIB ------- OBIB, indented with text labels

SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

MAX -------- Same as ALL
PATS ------- PI, SO
SCAN ------- TI and FCRD (random display, no answer number. SCAN must be entered on the same line as DISPLAY, e.g., D SCAN.)
SSRX ------- Single-Step Reactions (Map, Diagram, and Summary for all single-step reactions)
STD -------- BIB, IPC, and NCL

CRD -------- Compact Display of All Hit Reactions
CRDREF ----- Compact Reaction Display and SO, PY for Reference
FHIT ------- Reaction Map, Diagram, and Summary for first hit reaction
FHITCBIB --- FHIT, AN plus CBIB
FCRD ------- First hit in Compact Reaction Display (CRD) format
FCRDREF ---- First hit in Compact Reaction Display (CRD) format with CA reference information (SO, PY). (Default)
FPATH ------ PATH, plus Reaction Summary for the "long path"
FSPATH ----- SPATH, plus Reaction Summary for the "short path"
HIT -------- Reaction Map, Reaction Diagram, and Reaction Summary for all hit reactions and fields containing hit terms
OCC -------- All hit fields and the number of occurrences of the hit terms in each field. Includes total number of HIT, PATH, SPATH reactions. Labels reactions that have incomplete verifications.
PATH ------- Reaction Map and Reaction Diagram for the "long path". Displays all hit reactions, except those whose steps are totally included within another hit reaction which is displayed
RX --------- Hit Reactions (Map, Diagram, Summary for all hit reactions)
RXG -------- Hit Reaction Graphics (Map and Diagram for all hit reactions)
RXL -------- Hit Reaction Long (Map, Diagram, Summary for all hit reactions)

RXS -------- Hit Reaction Summariers (Map and Summary for all hit reactions)
SPATH ------ Reaction Map and Reaction Diagram for the "short path". Displays all single step reactions which contain a hit substance. Also displays those multistep reactions that have a hit substance in both the first and last steps of the reaction, except for those hit reactions whose steps are totally included within another hit reaction which is displayed

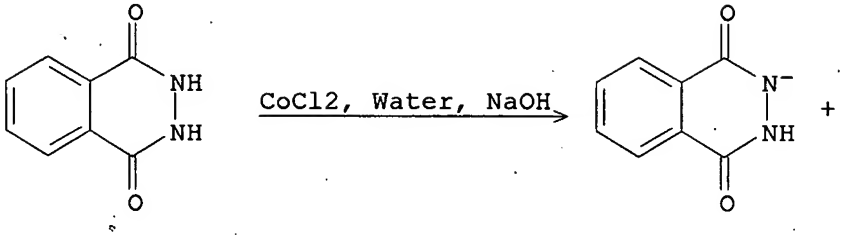
To display a particular field or fields, enter the display field codes. For a list of the display field codes, enter HELP DFIELDS at an arrow prompt (=>). Examples of combinations include: D TI; D BIB RX; D TI, AU, FCRD. The information is displayed in the same order as the specification. All of the formats, except CRD, CRDREF, FHIT, PATH, FPATH, SPATH, FSPATH, FCRD, FCRDREF, HIT, RX, RXG, RXS, SCAN, and OCC, may be used with the DISPLAY command to display the record for a specified Accession Number.

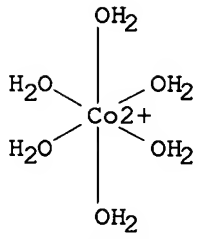
ENTER DISPLAY FORMAT (FCRDREF):END

=> D IBIB ABS CRD 1

L8 ANSWER 1 OF 103 CASREACT COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 148:91520 CASREACT
TITLE: X-ray crystal structure and vibrational spectra of hydrazides and their metal complexes. Part II. Hexaaquacobalt(II)bis(phthalhydrazidato)tetrahydrate
AUTHOR(S): Morzyk-Ociepa, Barbara
CORPORATE SOURCE: Institute of Chemistry and Environmental Protection, Jan Dlugosz University, Czestochowa, 42-200, Pol.
SOURCE: Journal of Molecular Structure (2007), 846(1-3), 74-86
CODEN: JMOSB4; ISSN: 0022-2860
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The hexaaquacobalt(II) bis(phthalhydrazidate) tetrahydrate, [Co(H2O)6](C8N2O2H5)2·4H2O, was examined using single crystal x-ray diffraction anal. The crystals are triclinic, space group P.hivin.1, with a 9.757(1), b 10.955(2), c 11.106(1) , α 100.79(2), β 90.35(3), γ 91.54(1)° and Z = 2. In [Co(H2O)6](C8N2O2H5)2·4H2O, the Co(II) is coordinated by six H2O ligands and the [Co(H2O)6]2+ is associated with the two O-deprotonated phthalhydrazidato ions only by H bonds. The IR and Raman spectra of phthalhydrazide (PH) and IR spectra of deuterated derivative phthalhydrazide (PD) and of [Co(H2O)6](C8N2O2H5)2·4H2O are reported. The theor. wavenumbers, IR intensities and Raman scattering activities were calculated using d. functional (B3LYP) method with the 6-311++G(d,p) basis set. The calculated potential energy distribution proved to be of great help in assigning the spectra of PH, its deuterated derivative and [Co(H2O)6](C8N2O2H5)2·4H2O. The results from natural bond orbital (NBO) anal. for the keto-hydroxy form of PH are presented.

RX(1) OF 2




CON: STAGE(1) room temperature; room temperature -> 318 deg C;
2 weeks, room temperature

REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> FIL REG

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| FULL ESTIMATED COST | 136.76 | 136.97 |

| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| CA SUBSCRIBER PRICE | -0.75 | -0.75 |

FILE 'REGISTRY' ENTERED AT 10:10:03 ON 16 JUL 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.


Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 15 JUL 2008 HIGHEST RN 1034171-01-1
DICTIONARY FILE UPDATES: 15 JUL 2008 HIGHEST RN 1034171-01-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information

on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=> D HIS

(FILE 'HOME' ENTERED AT 10:01:41 ON 16 JUL 2008)

FILE 'CASREACT' ENTERED AT 10:02:07 ON 16 JUL 2008
L1 STRUCTURE UPLOADED
L2 50 S L1
L3 STRUCTURE UPLOADED
L4 50 S L3
L5 0 S L4 AND ?DEUTERAT?
L6 17407 S L3 FUL
L7 16789 S L6/COM
L8 103 S L7 AND ?DEUTERAT?

FILE 'REGISTRY' ENTERED AT 10:10:03 ON 16 JUL 2008

=> FIL CAP

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| FULL ESTIMATED COST | 0.46 | 137.43 |

| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| CA SUBSCRIBER PRICE | 0.00 | -0.75 |

FILE 'CAPLUS' ENTERED AT 10:10:31 ON 16 JUL 2008
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FILE COVERS 1907 - 16 Jul 2008 VOL 149 ISS 3
FILE LAST UPDATED: 15 Jul 2008 (20080715/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/legal/infopolicy.html

=> E DEUTERATION/CT
E# FREQUENCY AT TERM

```
--    ---------     --      ----
E1            0      1      DEUTERATED/CT
E2            0      2      DEUTERATED POLYETHYLENE FIBERS/CT
E3         2123      6 --> DEUTERATION/CT
E4            0      2      DEUTERATION (L) ENTHALPY/CT
E5            0      5      DEUTERATION (L) REGIOSELECTIVE/CT
E6            0      6      DEUTERATION (L) STEREOSELECTIVE/CT
E7            0      2      DEUTERATION CATALYST/CT
E8          293      5      DEUTERATION CATALYSTS/CT
E9            2      9      DEUTERATION ENTHALPY/CT
E10          43      5      DEUTERATION KINETICS/CT
E11           0     12      DEUTERIDE/CT
E12           0     10      DEUTERIUM/CT

=> E E3+ALL
E1        28768   BT1  Reaction/CT
E2         2123     -->  Deuteration/CT
                      HNTE Valid heading during volume 76 (1972) to present.
E3          293       RT   Deuteration catalysts/CT
E4           43       RT   Deuteration kinetics/CT
E5         7182       RT   Proton transfer/CT
E6         9684       RT   Protonation/CT
********** END **********

=> S DEUTERATION+PFT/CT
L9         2123 DEUTERATION+PFT/CT  (1 TERM)

=> E US2007-521531/APPS
E1            1      US2007-5210/AP
E2            2      US2007-5211/AP
E3            1 --> US2007-521531/AP
E4            0      US2007-521531/PRN
E5            1      US2007-521619/AP
E6            1      US2007-522106/AP
E7            1      US2007-5226/AP
E8            1      US2007-523933/AP
E9            1      US2007-5243/AP
E10           1      US2007-524672/AP
E11           1      US2007-5250/AP
E12           1      US2007-5252/AP

=> S E3
L10           1 US2007-521531/AP

=> D SCA

L10   1 ANSWERS   CAPLUS  COPYRIGHT 2008 ACS on STN
IC    ICM  C07B059-00
      ICS  C07C005-00; C07C015-16; C07C037-00; C07C039-04; C07C039-28;
           C07C051-347; C07C063-06; C07C063-08; C07C209-68; C07C211-46;
           C07C217-84; C07C315-04; C07C317-14; C07M005-00
CC    25-1 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
TI    Process for preparation of deuterated aromatic compounds
ST    prepn deuterated arom compd deuteration catalyst
IT    Deuteration
      Deuteration catalysts
      Tritiation
      Tritiation catalysts
```

(preparation of deuterated aromatic compds.)
IT Aromatic compounds
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of deuterated aromatic compds.)
IT 62-53-3DP, Aniline, deuterated on para- and ortho-positions 7329-50-2P, Phen-2,4,6-d3-ol
RL: BYP (Byproduct); PREP (Preparation)
(preparation of deuterated aromatic compds.)
IT 7440-02-0, Nickel, uses 7440-06-4, Platinum, uses 7440-16-6, Rhodium, uses 7440-18-8, Ruthenium, uses 7440-48-4, Cobalt, uses 10025-99-7, Platinous potassium chloride
RL: CAT (Catalyst use); USES (Uses)
(preparation of deuterated aromatic compds.)
IT 62-53-3, Aniline, reactions 65-85-0, Benzoic acid, reactions 95-54-5, 1,2-Phenylenediamine, reactions 101-81-5, Diphenylmethane 102-51-2, 4-Methoxy-1,2-phenylenediamine 108-43-0, 3-Chlorophenol 108-95-2, Phenol, reactions 127-63-9, Diphenylsulfone 139-66-2, Diphenyl sulfide 532-32-1, Benzoic acid sodium salt 945-51-7, Diphenyl sulfoxide 7789-20-0, Deuterium oxide
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of deuterated aromatic compds.)
IT 101-81-5DP, Diphenylmethane, deuterated on Ph ring 108-43-0DP, 3-Chlorophenol, deuterated 127-63-9DP, Diphenylsulfone, deuterated 532-32-1DP, Sodium benzoate, deuterated 1079-02-3P, Benzoic-d5 acid 4165-61-1P, Benzen-d5-amine 4165-62-2P, Phen-d5-ol 35782-14-0P 62790-26-5P 74383-28-1DP, deuterated 87976-31-6DP, Benzoic-3,4,5-d3 acid, deuterated 291765-93-0P, 1,2-Benzene-3,4,5,6-d4-diamine 654062-93-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of deuterated aromatic compds.)

ALL ANSWERS HAVE BEEN SCANNED

=> SEL RN
E1 THROUGH E28 ASSIGNED

=> FIL REG

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| FULL ESTIMATED COST | 5.29 | 142.72 |

| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| CA SUBSCRIBER PRICE | 0.00 | -0.75 |

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DICTIONARY FILE UPDATES: 15 JUL 2008 HIGHEST RN 1034171-01-1

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TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

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http://www.cas.org/support/stngen/stndoc/properties.html

=> S E1-28

1 101-81-5/BI
(101-81-5/RN)
1 108-43-0/BI
(108-43-0/RN)
1 127-63-9/BI
(127-63-9/RN)
1 532-32-1/BI
(532-32-1/RN)
1 62-53-3/BI
(62-53-3/RN)
1 10025-99-7/BI
(10025-99-7/RN)
1 102-51-2/BI
(102-51-2/RN)
1 1079-02-3/BI
(1079-02-3/RN)
1 108-95-2/BI
(108-95-2/RN)
1 139-66-2/BI
(139-66-2/RN)
1 291765-93-0/BI
(291765-93-0/RN)
1 35782-14-0/BI
(35782-14-0/RN)
1 4165-61-1/BI
(4165-61-1/RN)
1 4165-62-2/BI
(4165-62-2/RN)
1 62790-26-5/BI
(62790-26-5/RN)
1 65-85-0/BI
(65-85-0/RN)
1 654062-93-8/BI
(654062-93-8/RN)
1 7329-50-2/BI
(7329-50-2/RN)
1 74383-28-1/BI
(74383-28-1/RN)
1 7440-02-0/BI
(7440-02-0/RN)
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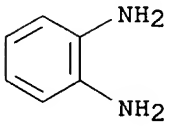
(7440-06-4/RN)
1 7440-16-6/BI

(7440-16-6/RN)
1 7440-18-8/BI
(7440-18-8/RN)
1 7440-48-4/BI
(7440-48-4/RN)
1 7789-20-0/BI
(7789-20-0/RN)
1 87976-31-6/BI
(87976-31-6/RN)
1 945-51-7/BI
(945-51-7/RN)
1 95-54-5/BI
(95-54-5/RN)
L11 28 (101-81-5/BI OR 108-43-0/BI OR 127-63-9/BI OR 532-32-1/BI OR 62-53-3/BI OR 10025-99-7/BI OR 102-51-2/BI OR 1079-02-3/BI OR 108-95-2/BI OR 139-66-2/BI OR 291765-93-0/BI OR 35782-14-0/BI OR 4165-61-1/BI OR 4165-62-2/BI OR 62790-26-5/BI OR 65-85-0/BI OR 654062-93-8/BI OR 7329-50-2/BI OR 74383-28-1/BI OR 7440-02-0/BI OR 7440-06-4/BI OR 7440-16-6/BI OR 7440-18-8/BI OR 7440-48-4/BI OR 7789-20-0/BI OR 87976-31-6/BI OR 945-51-7/BI OR 95-54-5/BI)

=> D SCA

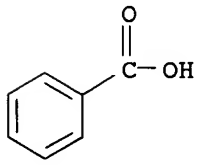
L11 28 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 1,2-Benzenediamine
MF C6 H8 N2
CI COM




**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

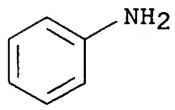
L11 28 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN Benzoic acid
MF C7 H6 O2
CI COM




**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

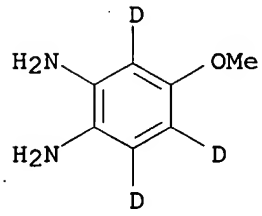
L11 28 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN Benzenamine
MF C6 H7 N
CI COM




**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L11 28 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 1,2-Benzene-3,4,6-d3-diamine, 5-methoxy- (9CI)
MF C7 H7 D3 N2 O




HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):END

=> FIL REG

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| FULL ESTIMATED COST | 0.46 | 143.18 |

| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| CA SUBSCRIBER PRICE | 0.00 | -0.75 |

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STRUCTURE FILE UPDATES: 15 JUL 2008 HIGHEST RN 1034171-01-1
DICTIONARY FILE UPDATES: 15 JUL 2008 HIGHEST RN 1034171-01-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

```
=> STR
:GRA C2
:ARR
:DIS

C~~C
1   2

:NOD 1 CY,2 D
:DIS

Cy~~D
1   2

:GGC 1 UNS
:END
L12  STRUCTURE CREATED

=> S L12
SAMPLE SEARCH INITIATED 10:12:12 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -  1808767 TO ITERATE

  0.1% PROCESSED     2000 ITERATIONS                          50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **INCOMPLETE**
PROJECTED ITERATIONS:     36111421 TO 36239259
PROJECTED ANSWERS:        30579072 TO 30701952

L13          50 SEA SSS SAM L12

=> SCR 2039
L14  SCREEN CREATED

=> D HSI
L14 HAS NO ANSWERS
L14             SCR 2039
```

```
=> D HIS

     (FILE 'HOME' ENTERED AT 10:01:41 ON 16 JUL 2008)

     FILE 'CASREACT' ENTERED AT 10:02:07 ON 16 JUL 2008
L1              STRUCTURE UPLOADED
L2           50 S L1
L3              STRUCTURE UPLOADED
L4           50 S L3
L5            0 S L4 AND ?DEUTERAT?
L6        17407 S L3 FUL
L7        16789 S L6/COM
L8          103 S L7 AND ?DEUTERAT?

     FILE 'REGISTRY' ENTERED AT 10:10:03 ON 16 JUL 2008

     FILE 'CAPLUS' ENTERED AT 10:10:31 ON 16 JUL 2008
                E DEUTERATION/CT
                E E3+ALL
L9         2123 S DEUTERATION+PFT/CT
                E US2007-521531/APPS
L10           1 S E3
                SEL RN

     FILE 'REGISTRY' ENTERED AT 10:11:28 ON 16 JUL 2008
L11          28 S E1-28

     FILE 'REGISTRY' ENTERED AT 10:11:51 ON 16 JUL 2008
L12             STR
L13          50 S L12
L14             SCR 2039

=> S L14 AND L12
SAMPLE SEARCH INITIATED 10:16:35 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -    14204 TO ITERATE

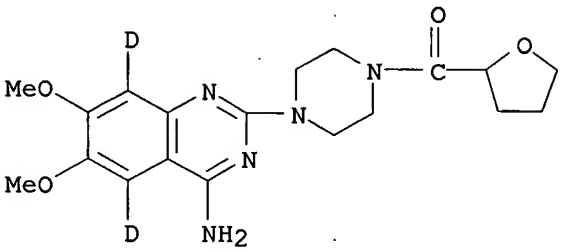
 14.1% PROCESSED     2000 ITERATIONS                                 50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       276940 TO   291220
PROJECTED ANSWERS:          161001 TO   171939

L15          50 SEA SSS SAM L14 AND L12

=> D SCA

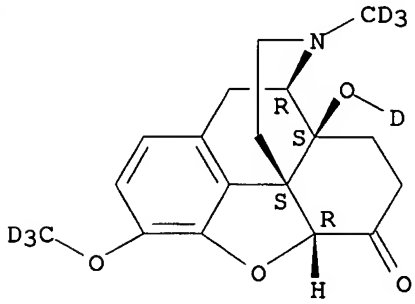
L15  50 ANSWERS   REGISTRY  COPYRIGHT 2008 ACS on STN
IN   Methanone, [4-(4-amino-6,7-dimethoxy-2-quinazolinyl-5,8-d2)-1-
     piperazinyl](tetrahydro-2-furanyl)-
MF   C19 H23 D2 N5 O4
```



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L15 50 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN Morphinan-6-one, 4,5-epoxy-14-(hydroxy-d)-3-(methoxy-d3)-17-(methyl-d3)-, (5α)-
MF C18 H14 D7 N O4

Absolute stereochemistry.



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):END

=> S L14 AND L12 FUL
FULL SEARCH INITIATED 10:16:48 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 281029 TO ITERATE

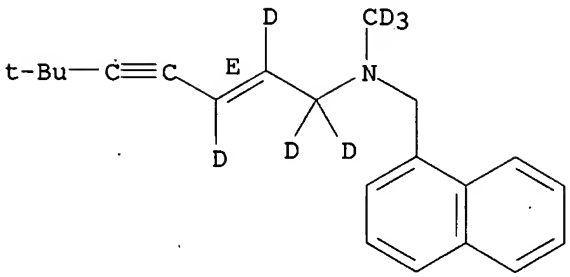
100.0% PROCESSED 281029 ITERATIONS 165475 ANSWERS
SEARCH TIME: 00.00.03

L16 165475 SEA SSS FUL L14 AND L12

=> D SCA

L16 165475 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN INDEX NAME NOT YET ASSIGNED
MF C21 H18 D7 N

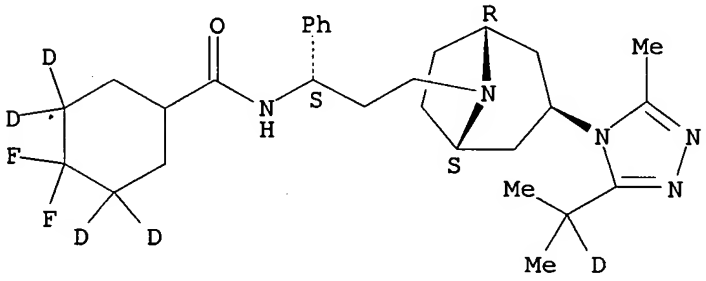
Double bond geometry as shown.



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L16 165475 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN INDEX NAME NOT YET ASSIGNED
MF C29 H36 D5 F2 N5 O

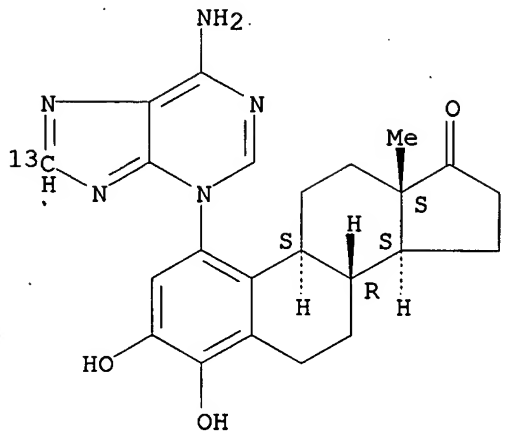
Absolute stereochemistry.



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L16 165475 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN INDEX NAME NOT YET ASSIGNED
MF C23 H25 N5 O3

Absolute stereochemistry.




HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):END

=> D HIS

(FILE 'HOME' ENTERED AT 10:01:41 ON 16 JUL 2008)

FILE 'CASREACT' ENTERED AT 10:02:07 ON 16 JUL 2008
L1 STRUCTURE UPLOADED
L2 50 S L1
L3 STRUCTURE UPLOADED
L4 50 S L3
L5 0 S L4 AND ?DEUTERAT?
L6 17407 S L3 FUL
L7 16789 S L6/COM
L8 103 S L7 AND ?DEUTERAT?

FILE 'REGISTRY' ENTERED AT 10:10:03 ON 16 JUL 2008

FILE 'CAPLUS' ENTERED AT 10:10:31 ON 16 JUL 2008
E DEUTERATION/CT
E E3+ALL
L9 2123 S DEUTERATION+PFT/CT
E US2007-521531/APPS
L10 1 S E3
SEL RN

FILE 'REGISTRY' ENTERED AT 10:11:28 ON 16 JUL 2008
L11 28 S E1-28

FILE 'REGISTRY' ENTERED AT 10:11:51 ON 16 JUL 2008
L12 STR
L13 50 S L12
L14 SCR 2039
L15 50 S L14 AND L12
L16 165475 S L14 AND L12 FUL

=> STR
:GRA C1
:DIS

```
C 1

:GRA C1,C1,C1,C1,C1
:ARR
:DIS
C 1      C 2      C 3      C 4      C 5      C 6

:NOD 2 PT,3 RH,4 RO,T NI,6 CO
ELEMENT SYMBOL NOT VALID
An element symbol specified is not valid.  Enter "HELP NODE" for more
information.
:DIS
C 1      Pt 2     Rh 3     C 4      C 5      C 6

:NOD 4 RO,5 NI,6 CO
ELEMENT SYMBOL NOT VALID
An element symbol specified is not valid.  Enter "HELP NODE" for more
information.
:NOD 4 RU,5 NI,6 CO
:DIS
C 1      Pt 2     Rh 3     Ru 4     Ni 5     Co 6

:NOD 1 G1
:NSP 2 3 4 5 6 RC
:VAR G1=2/3/4/5/6
:DIS
G1 1     Pt @2    Rh @3    Ru @4    Ni @5    Co @6

VAR G1=2/3/4/5/6
:END
L17  STRUCTURE CREATED

=> D HIS

     (FILE 'HOME' ENTERED AT 10:01:41 ON 16 JUL 2008)

     FILE 'CASREACT' ENTERED AT 10:02:07 ON 16 JUL 2008
L1              STRUCTURE UPLOADED
L2           50 S L1
L3              STRUCTURE UPLOADED
L4           50 S L3
L5            0 S L4 AND ?DEUTERAT?
L6        17407 S L3 FUL
L7        16789 S L6/COM
L8          103 S L7 AND ?DEUTERAT?

     FILE 'REGISTRY' ENTERED AT 10:10:03 ON 16 JUL 2008

     FILE 'CAPLUS' ENTERED AT 10:10:31 ON 16 JUL 2008
                E DEUTERATION/CT
                E E3+ALL
L9         2123 S DEUTERATION+PFT/CT
                E US2007-521531/APPS
```

```
L10             1 S E3
                  SEL RN

     FILE 'REGISTRY' ENTERED AT 10:11:28 ON 16 JUL 2008
L11            28 S E1-28

     FILE 'REGISTRY' ENTERED AT 10:11:51 ON 16 JUL 2008
L12               STR
L13            50 S L12
L14               SCR 2039
L15            50 S L14 AND L12
L16        165475 S L14 AND L12 FUL
L17               STR

=> FIL CAP
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                     183.42     326.60

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                         ENTRY    SESSION
CA SUBSCRIBER PRICE                                       0.00      -0.75

FILE 'CAPLUS' ENTERED AT 10:19:09 ON 16 JUL 2008
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FILE COVERS 1907 - 16 Jul 2008  VOL 149 ISS 3
FILE LAST UPDATED: 15 Jul 2008  (20080715/ED)

Caplus now includes complete International Patent Classification (IPC)
reclassification data for the second quarter of 2008.

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/legal/infopolicy.html

=> S L16 AND L9
         69206 L16
L18       1004 L16 AND L9

=> FIL REG
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                       0.48     327.08
```

```
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)        SINCE FILE      TOTAL
                                                     ENTRY    SESSION
CA SUBSCRIBER PRICE                                   0.00      -0.75

FILE 'REGISTRY' ENTERED AT 10:20:02 ON 16 JUL 2008
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STRUCTURE FILE UPDATES:   15 JUL 2008  HIGHEST RN 1034171-01-1
DICTIONARY FILE UPDATES:  15 JUL 2008  HIGHEST RN 1034171-01-1

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  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=> TRA L18 RN
SELECT IS APPROXIMATELY 96% COMPLETE
L19          TRANSFER L18 1- RN :    17055 TERMS
SEARCH OF L19 IS APPROXIMATELY 41% COMPLETE
SEARCH OF L19 IS APPROXIMATELY 78% COMPLETE
L20       17055 L19

=> D HIS


     (FILE 'HOME' ENTERED AT 10:01:41 ON 16 JUL 2008)

     FILE 'CASREACT' ENTERED AT 10:02:07 ON 16 JUL 2008
L1              STRUCTURE UPLOADED
L2           50 S L1
L3              STRUCTURE UPLOADED
L4           50 S L3
L5            0 S L4 AND ?DEUTERAT?
L6        17407 S L3 FUL
L7        16789 S L6/COM
L8          103 S L7 AND ?DEUTERAT?

     FILE 'REGISTRY' ENTERED AT 10:10:03 ON 16 JUL 2008

     FILE 'CAPLUS' ENTERED AT 10:10:31 ON 16 JUL 2008
                E DEUTERATION/CT
                E E3+ALL
L9          2123 S DEUTERATION+PFT/CT
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                E US2007-521531/APPS
L10           1 S E3
                SEL RN

     FILE 'REGISTRY' ENTERED AT 10:11:28 ON 16 JUL 2008
L11          28 S E1-28

     FILE 'REGISTRY' ENTERED AT 10:11:51 ON 16 JUL 2008
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L13          50 S L12
L14             SCR 2039
L15          50 S L14 AND L12
L16      165475 S L14 AND L12 FUL
L17             STR

     FILE 'CAPLUS' ENTERED AT 10:19:09 ON 16 JUL 2008
L18        1004 S L16 AND L9

     FILE 'REGISTRY' ENTERED AT 10:20:02 ON 16 JUL 2008

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L19             TRA L18 1- RN :    17055 TERMS

     FILE 'REGISTRY' ENTERED AT 10:20:38 ON 16 JUL 2008
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=> S L17 SUB=L20 SAM
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SAMPLE SUBSET SCREEN SEARCH COMPLETED -       34 TO ITERATE

100.0% PROCESSED       34 ITERATIONS                          27 ANSWERS
SEARCH TIME: 00.00.01

PROJECTIONS (WITHIN SPECIFIED SUBSET):          ONLINE  **COMPLETE**
PROJECTED ITERATIONS (WITHIN SPECIFIED SUBSET):         331 TO     1029
PROJECTED ANSWERS (WITHIN SPECIFIED SUBSET):            229 TO      851

L21           27 SEA SUB=L20 SSS SAM L17

=> S L17 SUB=L20 FUL
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FULL SUBSET SCREEN SEARCH COMPLETED -      511 TO ITERATE

100.0% PROCESSED      511 ITERATIONS                         449 ANSWERS
SEARCH TIME: 00.00.01

L22          449 SEA SUB=L20 SSS FUL L17

=> D SCA

L22  449 ANSWERS   REGISTRY  COPYRIGHT 2008 ACS on STN
IN   Ruthenium(2+), (2,2'-bipyridine-3,3',4,4',5,5',6,6'-d8-
     κN1,κN1')bis[4,7-di(phenyl-2,3,4,5,6-d5)-1,10-phenanthroline-
     2,3,5,6,8,9-d6-κN1,κN10]-, (OC-6-22)-, hexafluorophosphate(1-)
     (1:2)
MF   C58 D40 N6 Ru . 2 F6 P

     CM   1
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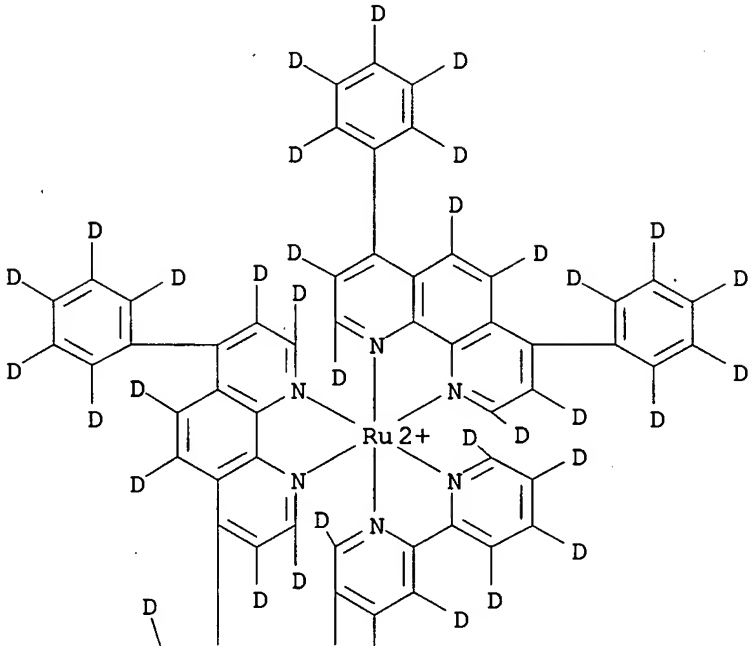
PAGE 1-A



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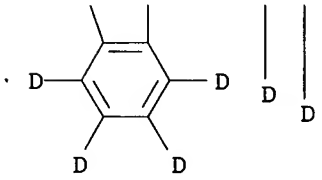

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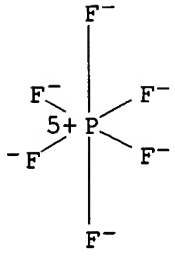

**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

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HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):END

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L2           50 S L1
L3              STRUCTURE UPLOADED
L4           50 S L3
L5            0 S L4 AND ?DEUTERAT?
L6        17407 S L3 FUL
L7        16789 S L6/COM
L8          103 S L7 AND ?DEUTERAT?

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                E E3+ALL
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                E US2007-521531/APPS
L10            1 S E3
                SEL RN

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     FILE 'REGISTRY' ENTERED AT 10:11:51 ON 16 JUL 2008
L12             STR
L13          50 S L12
L14             SCR 2039
L15          50 S L14 AND L12
L16      165475 S L14 AND L12 FUL
L17             STR

     FILE 'CAPLUS' ENTERED AT 10:19:09 ON 16 JUL 2008
L18        1004 S L16 AND L9

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     FILE 'CAPLUS' ENTERED AT 10:20:06 ON 16 JUL 2008
L19             TRA L18 1- RN :    17055 TERMS

     FILE 'REGISTRY' ENTERED AT 10:20:38 ON 16 JUL 2008
L20       17055 SEA L19
L21          27 S L17 SAM SUB=L20
L22         449 S L17 FUL SUB=L20

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COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                             179.28     518.95

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)    SINCE FILE      TOTAL
                                                 ENTRY    SESSION
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FILE COVERS 1907 - 16 Jul 2008 VOL 149 ISS 3
FILE LAST UPDATED: 15 Jul 2008 (20080715/ED)

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L5 0 S L4 AND ?DEUTERAT?
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L7 16789 S L6/COM
L8 103 S L7 AND ?DEUTERAT?

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E E3+ALL
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E US2007-521531/APPS
L10 1 S E3
SEL RN

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FILE 'REGISTRY' ENTERED AT 10:11:51 ON 16 JUL 2008
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L14             SCR 2039
L15          50 S L14 AND L12
L16      165475 S L14 AND L12 FUL
L17             STR

     FILE 'CAPLUS' ENTERED AT 10:19:09 ON 16 JUL 2008
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         118578 L22(L)CAT+NT/RL
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=> D IBIB ABS HITIND HITSTR 10

L23  ANSWER 10 OF 77  CAPLUS  COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:         2006:1169153  CAPLUS
DOCUMENT NUMBER:          147:234843
TITLE:                    Organic reaction in water: Part 10. Reduction of
                          biphenyl, naphthalene and acenaphthene with noble
                          Rh/C, Ru/C, Pd/C, Pt/C catalysts and Al powder in
                          deuterium oxide
AUTHOR(S):                Suzuki, Hiroshi; Tashiro, Hideki; Ishimoto, Keiko;
                          Prakash, G. K. Surya; Olah, George A.; Tashiro,
                          Masashi
CORPORATE SOURCE:         Loker Hydrocarbon Research Institute, University of
                          Southern California, Los Angeles, CA, 90089-1661, USA
SOURCE:                   Japanese Journal of Deuterium Science (2006), 12(1),
                          33-37
                          CODEN: JJDSFY; ISSN: 1343-0718
PUBLISHER:                Japanese Society for Deuterium Science
DOCUMENT TYPE:            Journal
LANGUAGE:                 English
AB   The hydrogenation of biphenyl and naphthalene was carried out with Rh/C,
     Ru/C, Pd/C Pt/C catalysts and Al powder in D2O in sealed tube.  In each
     case, overdeuterated compds. were obtained.  Treatment of cis- and
     trans-decalins with noble metal catalysts and Al powder in D2O afforded a
     mixture of deuterated decalins (no data).  This shows that H-D exchange
     reaction occurred in the treatment of aliphatic compds. with noble metal
     catalysts and Al powder in D2O solution  Also pure dicyclohexane-d22, cis-,
     trans-decalins-d18 and decahydroacenaphtene-d20 were obtained from
     deuterated biphenyl-d10, naphthalene-d8 and acenaphthene-d10 (no data).
CC   25-24 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
IT   Deuteration
```

Deuteration catalysts
Reduction
Reduction catalysts
(reduction of biphenyl, naphthalene and acenaphthene with noble Rh/C, Ru/C, Pd/C, Pt/C catalysts and Al powder in deuterium oxide)

IT 7429-90-5, Aluminum, uses 7440-05-3, Palladium, uses 7440-06-4, Platinum, uses 7440-16-6, Rhodium, uses 7440-18-8, Ruthenium, uses 7440-44-0, Carbon, uses
RL: CAT (Catalyst use); USES (Uses)
(reduction of biphenyl, naphthalene and acenaphthene with noble Rh/C, Ru/C, Pd/C, Pt/C catalysts and Al powder in deuterium oxide)

IT 91-20-3, Naphthalene, reactions 92-52-4, 1,1'-Biphenyl, reactions 1146-65-2, Naphthalene-d8
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction of biphenyl, naphthalene and acenaphthene with noble Rh/C, Ru/C, Pd/C, Pt/C catalysts and Al powder in deuterium oxide)

IT 7440-06-4, Platinum, uses 7440-16-6, Rhodium, uses 7440-18-8, Ruthenium, uses
RL: CAT (Catalyst use); USES (Uses)
(reduction of biphenyl, naphthalene and acenaphthene with noble Rh/C, Ru/C, Pd/C, Pt/C catalysts and Al powder in deuterium oxide)

RN 7440-06-4 CAPLUS
CN Platinum (CA INDEX NAME)

Pt

RN 7440-16-6 CAPLUS
CN Rhodium (CA INDEX NAME)

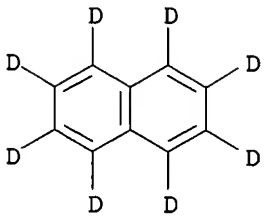
Rh

RN 7440-18-8 CAPLUS
CN Ruthenium (CA INDEX NAME)

Ru

IT 1146-65-2, Naphthalene-d8
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction of biphenyl, naphthalene and acenaphthene with noble Rh/C, Ru/C, Pd/C, Pt/C catalysts and Al powder in deuterium oxide)

RN 1146-65-2 CAPLUS
CN Naphthalene-1,2,3,4,5,6,7,8-d8 (CA INDEX NAME)




REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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(FILE 'HOME' ENTERED AT 10:01:41 ON 16 JUL 2008)

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L2 50 S L1
L3 STRUCTURE UPLOADED
L4 50 S L3
L5 0 S L4 AND ?DEUTERAT?
L6 17407 S L3 FUL
L7 16789 S L6/COM
L8 103 S L7 AND ?DEUTERAT?

FILE 'REGISTRY' ENTERED AT 10:10:03 ON 16 JUL 2008

FILE 'CAPLUS' ENTERED AT 10:10:31 ON 16 JUL 2008
E DEUTERATION/CT
E E3+ALL
L9 2123 S DEUTERATION+PFT/CT
E US2007-521531/APPS
L10 1 S E3
SEL RN

FILE 'REGISTRY' ENTERED AT 10:11:28 ON 16 JUL 2008
L11 28 S E1-28

FILE 'REGISTRY' ENTERED AT 10:11:51 ON 16 JUL 2008
L12 STR
L13 50 S L12
L14 SCR 2039
L15 50 S L14 AND L12
L16 165475 S L14 AND L12 FUL
L17 STR

FILE 'CAPLUS' ENTERED AT 10:19:09 ON 16 JUL 2008
L18 1004 S L16 AND L9

FILE 'REGISTRY' ENTERED AT 10:20:02 ON 16 JUL 2008

FILE 'CAPLUS' ENTERED AT 10:20:06 ON 16 JUL 2008
L19 TRA L18 1- RN : 17055 TERMS

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     FILE 'REGISTRY' ENTERED AT 10:20:38 ON 16 JUL 2008
L20        17055 SEA L19
L21           27 S L17 SAM SUB=L20
L22          449 S L17 FUL SUB=L20

     FILE 'CAPLUS' ENTERED AT 10:22:14 ON 16 JUL 2008
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         69206 L16
       4604203 PREP+NT/RL  (18 TERMS)
         40333 L16(L)PREP+NT/RL
L24         72 L23 AND L16(L)PREP+NT/RL

=> s l24 and l10
L25           1 L24 AND L10

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      1 ANSWERS ARE AVAILABLE.  SPECIFIED ANSWER NUMBER EXCEEDS ANSWER SET SIZE
The answer numbers requested are not in the answer set.
ENTER ANSWER NUMBER OR RANGE (1):end

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L24  ANSWER 50 OF 72  CAPLUS  COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:         1990:531636  CAPLUS
DOCUMENT NUMBER:          113:131636
ORIGINAL REFERENCE NO.:   113:22351a,22354a
TITLE:                    Preparation of deuterated naphthalenes, anilines,
                          m-toluidines, and anisoles by reductive dehalogenation
                          of the corresponding halogenated derivatives with
                          Raney copper-aluminum alloy in an alkaline deuterium
                          oxide solution
AUTHOR(S):                Tashiro, Masashi; Tsuzuki, Hirohisa; Tsukinoki,
                          Takehito; Mataka, Shuntaro; Nakayama, Kouji;
                          Yonemitsu, Tadashi
CORPORATE SOURCE:         Inst. Adv. Mater. Study, Kyushu Univ., Kasuga, 816,
                          Japan
SOURCE:                   Journal of Labelled Compounds and Radiopharmaceuticals
                          (1990), 28(6), 703-12
                          CODEN: JLCRD4; ISSN: 0362-4803
DOCUMENT TYPE:            Journal
LANGUAGE:                 English
OTHER SOURCE(S):          CASREACT 113:131636
AB   Four deuterated naphthalenes, 10 deuterated anilines, 3 deuterated
     m-toluidine derivs., and 5 deuterated anisoles were prepared in high
     isotopic purities from the corresponding bromo or chloro precursors by
     reductive dehalogenation with Raney Cu-Al alloy in D2O containing NaOD.  E.g.,
     2-BrC6H4NH2 gave 75% 2-DC6H4NH2 in 97% isotopic purity.
CC   25-4 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
IT   Deuteration
        (of bromonaphthalenes, bromo- and chloroanilines, and bromoanisoles
        with sodium deuteroxide-deuterium oxide, Raney copper-aluminum
        alloy-catalyzed)
IT   11101-28-3
     RL: CAT (Catalyst use); USES (Uses)
        (Raney catalyst, for deuteration of bromonaphthalenes, bromo- and
        chloroaniline derivs., and bromoanisole derivs.)
```

IT 875-62-7P, 1-Deuterionaphthalene 1683-99-4P,
1-Amino-2,4-dideuterionaphthalene 2430-34-4P,
2-Deuterionaphthalene 2567-25-1P, 2,4,6-Trideuterioanisole
7291-08-9P, 2,4,6-Trideuterioaniline 13122-28-6P,
4-Deuterioaniline 19617-82-4P, 3,5-Dideuterioaniline
19617-83-5P, 2,3,5,6-Tetradeuterioaniline 20938-43-6P,
4-Deuterioanisole 23878-49-1P, 1,5-Dideuterionaphthalene
26351-62-2P, 2-Deuterioanisole 50535-17-6P,
2-Deuterioaniline 50535-18-7P, 3-Deuterioaniline
68408-23-1P 120364-25-2P, 2,3-Dideuterioaniline
122258-85-9P, 2,4-Dideuterioaniline 129453-25-4P,
2,5-Dideuterioaniline 129453-26-5P, 2,6-Dideuterioaniline
129453-27-6P 129453-28-7P 129453-29-8P,
2,4-Dideuterioanisole 129453-30-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 11101-28-3
RL: CAT (Catalyst use); USES (Uses)
(Raney catalyst, for deuteration of bromonaphthalenes, bromo- and chloroaniline derivs., and bromoanisole derivs.)
RN 11101-28-3 CAPLUS
CN Copper alloy, nonbase, Cu,Ni (CA INDEX NAME)

| Component | Component Registry Number |
|---|---|
| Cu | 7440-50-8 |
| Ni | 7440-02-0 |

IT 875-62-7P, 1-Deuterionaphthalene 1683-99-4P,
1-Amino-2,4-dideuterionaphthalene 2430-34-4P,
2-Deuterionaphthalene 2567-25-1P, 2,4,6-Trideuterioanisole
7291-08-9P, 2,4,6-Trideuterioaniline 13122-28-6P,
4-Deuterioaniline 19617-82-4P, 3,5-Dideuterioaniline
19617-83-5P, 2,3,5,6-Tetradeuterioaniline 20938-43-6P,
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2-Deuterioaniline 50535-18-7P, 3-Deuterioaniline
68408-23-1P 120364-25-2P, 2,3-Dideuterioaniline
122258-85-9P, 2,4-Dideuterioaniline 129453-25-4P,
2,5-Dideuterioaniline 129453-26-5P, 2,6-Dideuterioaniline
129453-27-6P 129453-28-7P 129453-29-8P,
2,4-Dideuterioanisole 129453-30-1P
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(preparation of)
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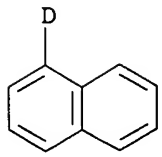
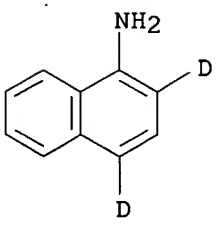
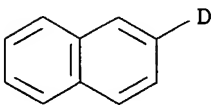
CN Naphthalene-1-d (CA INDEX NAME)




RN 1683-99-4 CAPLUS
CN 1-Naphthalen-2,4-d2-amine (9CI) (CA INDEX NAME)




RN 2430-34-4 CAPLUS
CN Naphthalene-2-d (CA INDEX NAME)

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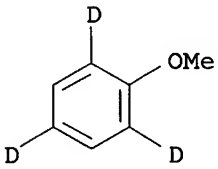
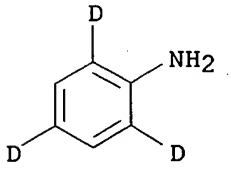
CN Benzene-1,3,5-d3, 2-methoxy- (9CI) (CA INDEX NAME)




RN 7291-08-9 CAPLUS
CN Benzen-2,4,6-d3-amine (9CI) (CA INDEX NAME)

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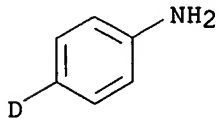
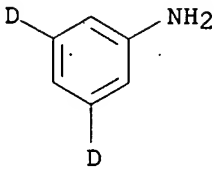
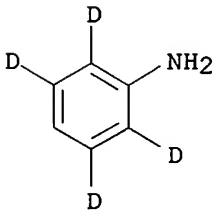



RN 19617-82-4 CAPLUS
CN Benzen-3,5-d2-amine (9CI) (CA INDEX NAME)



RN 19617-83-5 CAPLUS
CN Benzen-2,3,5,6-d4-amine (9CI) (CA INDEX NAME)



RN 20938-43-6 CAPLUS
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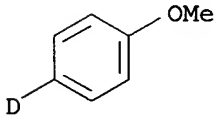

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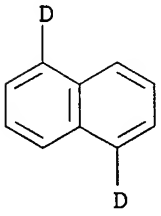
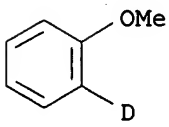


RN 26351-62-2 CAPLUS
CN Benzene-d, 2-methoxy- (9CI) (CA INDEX NAME)



RN 50535-17-6 CAPLUS
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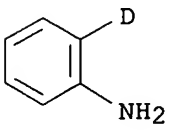

RN 50535-18-7 CAPLUS
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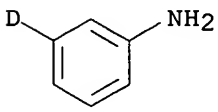

RN 68408-23-1 CAPLUS
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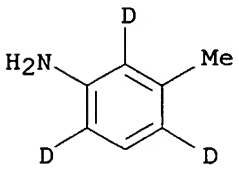

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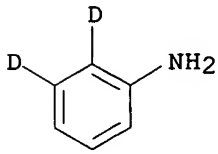

RN 122258-85-9 CAPLUS
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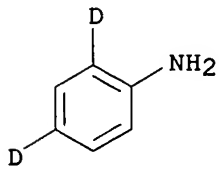

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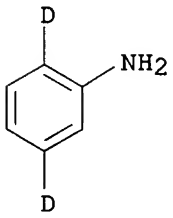

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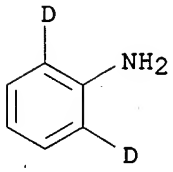

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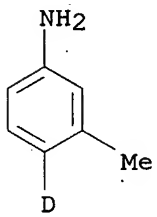
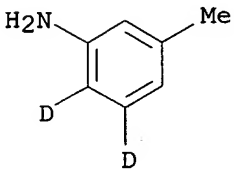


RN 129453-28-7 CAPLUS
CN Benzen-2,3-d2-amine, 5-methyl- (9CI) (CA INDEX NAME)



RN 129453-29-8 CAPLUS
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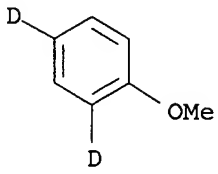


RN 129453-30-1 CAPLUS
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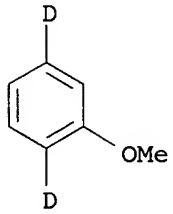


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(FILE 'HOME' ENTERED AT 10:01:41 ON 16 JUL 2008)

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L1 STRUCTURE UPLOADED
L2 50 S L1
L3 STRUCTURE UPLOADED
L4 50 S L3
L5 0 S L4 AND ?DEUTERAT?
L6 17407 S L3 FUL
L7 16789 S L6/COM
L8 103 S L7 AND ?DEUTERAT?

FILE 'REGISTRY' ENTERED AT 10:10:03 ON 16 JUL 2008

FILE 'CAPLUS' ENTERED AT 10:10:31 ON 16 JUL 2008
E DEUTERATION/CT
E E3+ALL
L9 2123 S DEUTERATION+PFT/CT
E US2007-521531/APPS
L10 1 S E3
SEL RN

FILE 'REGISTRY' ENTERED AT 10:11:28 ON 16 JUL 2008
L11 28 S E1-28

FILE 'REGISTRY' ENTERED AT 10:11:51 ON 16 JUL 2008
L12 STR
L13 50 S L12
L14 SCR 2039
L15 50 S L14 AND L12
L16 165475 S L14 AND L12 FUL

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L17             STR

     FILE 'CAPLUS' ENTERED AT 10:19:09 ON 16 JUL 2008
L18         1004 S L16 AND L9

     FILE 'REGISTRY' ENTERED AT 10:20:02 ON 16 JUL 2008

     FILE 'CAPLUS' ENTERED AT 10:20:06 ON 16 JUL 2008
L19             TRA L18 1- RN :    17055 TERMS

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L21            27 S L17 SAM SUB=L20
L22           449 S L17 FUL SUB=L20

     FILE 'CAPLUS' ENTERED AT 10:22:14 ON 16 JUL 2008
L23            77 S L22(L)CAT+NT/RL AND L18
L24            72 S L23 AND L16(L)PREP+NT/RL
L25             1 S L24 AND L10

=> d que l24
L9           2123 SEA FILE=CAPLUS DEUTERATION+PFT/CT
L12             STR

Cy~^D
 1   2


NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
GGCAT   IS UNS  AT   1
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS   2

STEREO ATTRIBUTES: NONE
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L16        165475 SEA FILE=REGISTRY SSS FUL L14 AND L12
L17             STR

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RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS   6

STEREO ATTRIBUTES: NONE
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=> d l24 ibib abs crd tot
'CRD' IS NOT A VALID FORMAT FOR FILE 'CAPLUS'

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ABS --------- GI and AB
ALL --------- BIB, AB, IND, RE
APPS -------- AI, PRAI
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CAN --------- List of CA abstract numbers without answer numbers
CBIB -------- AN, plus Compressed Bibliographic Data
CLASS ------- IPC, NCL, ECLA, FTERM
DALL -------- ALL, delimited (end of each field identified)
DMAX -------- MAX, delimited for post-processing
FAM --------- AN, PI and PRAI in table, plus Patent Family data
FBIB -------- AN, BIB, plus Patent FAM
IND --------- Indexing data
IPC --------- International Patent Classifications
MAX --------- ALL, plus Patent FAM, RE
PATS -------- PI, SO
SAM --------- CC, SX, TI, ST, IT
SCAN -------- CC, SX, TI, ST, IT (random display, no answer numbers;
              SCAN must be entered on the same line as the DISPLAY,
              e.g., D SCAN or DISPLAY SCAN)
STD --------- BIB, CLASS

IABS -------- ABS, indented with text labels
IALL -------- ALL, indented with text labels
IBIB -------- BIB, indented with text labels
IMAX -------- MAX, indented with text labels
ISTD -------- STD, indented with text labels

OBIB -------- AN, plus Bibliographic Data (original)
OIBIB ------- OBIB, indented with text labels

SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

HIT --------- Fields containing hit terms
HITIND ------ IC, ICA, ICI, NCL, CC and index field (ST and IT)
              containing hit terms
HITRN ------- HIT RN and its text modification
HITSTR ------ HIT RN, its text modification, its CA index name, and
              its structure diagram
HITSEQ ------ HIT RN, its text modification, its CA index name, its
              structure diagram, plus NTE and SEQ fields
FHITSTR ----- First HIT RN, its text modification, its CA index name, and
              its structure diagram
FHITSEQ ----- First HIT RN, its text modification, its CA index name, its
              structure diagram, plus NTE and SEQ fields
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KWIC -------- Hit term plus 20 words on either side
OCC --------- Number of occurrence of hit term and field in which it occurs

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ENTER DISPLAY FORMAT (BIB):end

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(FILE 'HOME' ENTERED AT 10:01:41 ON 16 JUL 2008)

FILE 'CASREACT' ENTERED AT 10:02:07 ON 16 JUL 2008
L1 STRUCTURE UPLOADED
L2 50 S L1
L3 STRUCTURE UPLOADED
L4 50 S L3
L5 0 S L4 AND ?DEUTERAT?
L6 17407 S L3 FUL
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L8 103 S L7 AND ?DEUTERAT?

FILE 'REGISTRY' ENTERED AT 10:10:03 ON 16 JUL 2008

FILE 'CAPLUS' ENTERED AT 10:10:31 ON 16 JUL 2008
E DEUTERATION/CT
E E3+ALL
L9 2123 S DEUTERATION+PFT/CT
E US2007-521531/APPS
L10 1 S E3
SEL RN

FILE 'REGISTRY' ENTERED AT 10:11:28 ON 16 JUL 2008
L11 28 S E1-28

FILE 'REGISTRY' ENTERED AT 10:11:51 ON 16 JUL 2008
L12 STR
L13 50 S L12
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L24           72 S L23 AND L16(L)PREP+NT/RL
L25            1 S L24 AND L10

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                                                       ENTRY    SESSION
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FILE COVERS 1907 - 16 Jul 2008  VOL 149 ISS 3
FILE LAST UPDATED: 15 Jul 2008  (20080715/ED)

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=> d que l24
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L12              STR

Cy~^D
 1   2


NODE ATTRIBUTES:
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GGCAT   IS UNS  AT   1
DEFAULT ECLEVEL IS LIMITED
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NUMBER OF NODES IS 2

STEREO ATTRIBUTES: NONE
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L17 STR

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VAR G1=2/3/4/5/6
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NSPEC IS RC AT 3
NSPEC IS RC AT 4
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NUMBER OF NODES IS 6

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L24 72 SEA FILE=CAPLUS L23 AND L16(L)PREP+NT/RL

=> d l24 ibib abs hitstr tot

L24 ANSWER 1 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2008:354069 CAPLUS
DOCUMENT NUMBER: 148:495347
TITLE: Efficient and selective Pt/C-catalyzed H-D exchange reaction of aromatic rings
AUTHOR(S): Ito, Nobuhiro; Esaki, Hiroyoshi; Maesawa, Tsuneaki; Imamiya, Eikoh; Maegawa, Tomohiro; Sajiki, Hironao
CORPORATE SOURCE: Chemical Products Research Laboratories, Wako Pure Chemical Industries, Ltd., Matoba, Kawagoe, 350-1101, Japan
SOURCE: Bulletin of the Chemical Society of Japan (2008), 81(2), 278-286
CODEN: BCSJA8; ISSN: 0009-2673
PUBLISHER: Chemical Society of Japan
DOCUMENT TYPE: Journal
LANGUAGE: English
AB An effective and applicable deuteration method for aromatic rings using Pt/C-D2O-H2 system was established. Especially, phenol was fully deuterated even at room temperature, and other electron-rich aromatic nuclei were efficiently deuterated under mild conditions. The scope and limitations of the presence method and its application to the synthesis of deuterium-labeled

biol. active compds. and deuterium-labeled building blocks for practical multi-gram scale syntheses are reported.

IT 7440-06-4, Platinum, uses
RL: CAT (Catalyst use); USES (Uses)
(selective Pt/C-catalyzed H/D exchange reaction of aromatic rings)

RN 7440-06-4 CAPLUS
CN Platinum (CA INDEX NAME)

Pt

IT 1079-02-3P, Benzoic-2,3,4,5,6-d5 acid 1486-01-7P
3947-98-6P 4165-61-1P, Benzen-2,3,4,5,6-d5-amine
4165-62-2P, Phen-2,3,4,5,6-d5-ol 103963-58-2P,
1,2-Benzene-3,4,5,6-d4-diol 121887-11-4P 124251-84-9P
291765-93-0P, 1,2-Benzene-3,4,5,6-d4-diamine 362049-56-7P
651316-68-6P, properties 861405-64-3P
868699-93-8P 868699-94-9P 931581-17-8P
1021325-35-8P 1021325-39-2P 1021325-40-5P
1021325-41-6P 1021325-42-7P 1021325-43-8P
1021325-44-9P 1021325-45-0P 1021325-46-1P
1021325-47-2P 1021325-48-3P 1021325-49-4P
1021325-50-7P 1021325-51-8P 1021325-52-9P
1021325-53-0P 1021325-54-1P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(selective Pt/C-catalyzed H/D exchange reaction of aromatic rings)

RN 1079-02-3 CAPLUS
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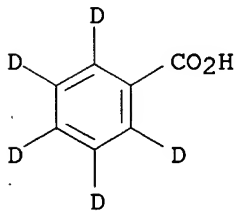


RN 1486-01-7 CAPLUS
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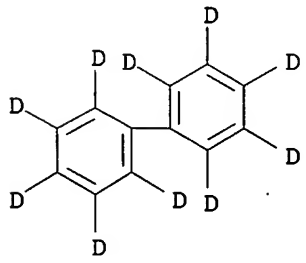


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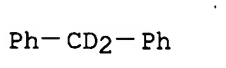

RN 4165-61-1 CAPLUS
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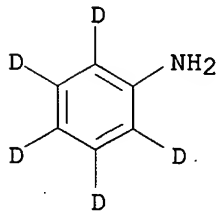

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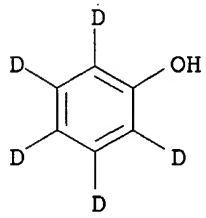

RN 103963-58-2 CAPLUS
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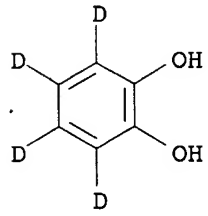

RN 121887-11-4 CAPLUS
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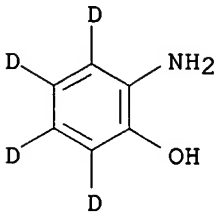

RN 124251-84-9 CAPLUS
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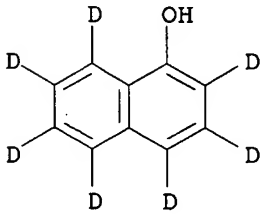
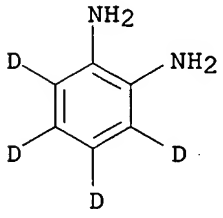
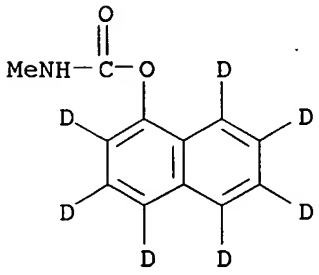


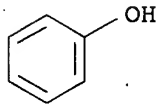
RN 291765-93-0 CAPLUS
CN 1,2-Benzene-3,4,5,6-d4-diamine (9CI) (CA INDEX NAME)



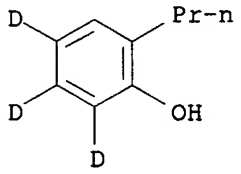
RN 362049-56-7 CAPLUS
CN 1-Naphthalen-2,3,4,5,6,7,8-d7-ol, methylcarbamate (9CI) (CA INDEX NAME)



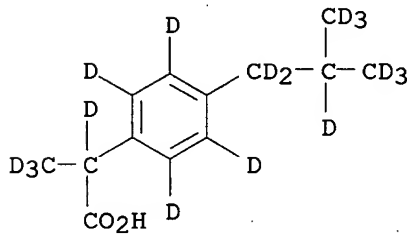
RN 651316-68-6 CAPLUS
CN Phenol, labeled with deuterium (9CI) (CA INDEX NAME)



RN 861405-64-3 CAPLUS
CN Phen-2,3,4-d3-ol, 6-propyl- (9CI) (CA INDEX NAME)

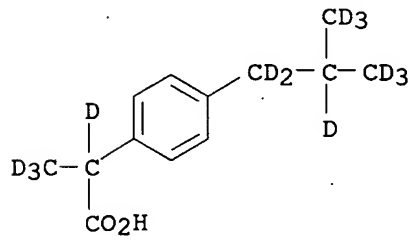


RN 868699-93-8 CAPLUS
CN Benzene-2,3,5,6-d4-acetic-α-d acid, α-(methyl-d3)-4-[2-(methyl-d3)propyl-1,1,2,3,3,3-d6]-, sodium salt (9CI) (CA INDEX NAME)



● Na

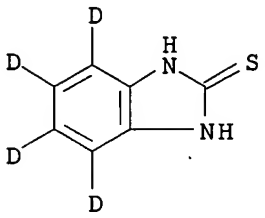
RN 868699-94-9 CAPLUS
CN Benzeneacetic-α-d acid, α-(methyl-d3)-4-[2-(methyl-d3)propyl-1,1,2,3,3,3-d6]-, sodium salt (1:1) (CA INDEX NAME)



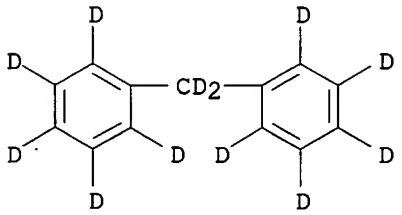
● Na

RN 931581-17-8 CAPLUS

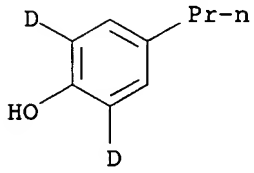
CN 2H-Benzimidazole-2-thione-4,5,6,7-d4, 1,3-dihydro- (CA INDEX NAME)



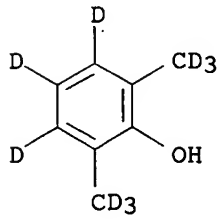
RN 1021325-35-8 CAPLUS
CN INDEX NAME NOT YET ASSIGNED



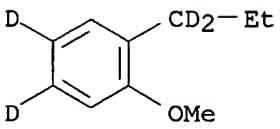
RN 1021325-39-2 CAPLUS
CN INDEX NAME NOT YET ASSIGNED



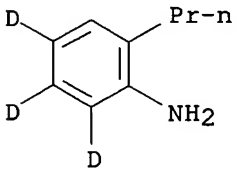
RN 1021325-40-5 CAPLUS
CN INDEX NAME NOT YET ASSIGNED



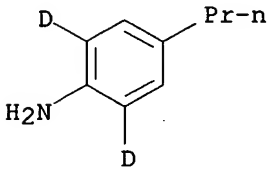
RN 1021325-41-6 CAPLUS
CN INDEX NAME NOT YET ASSIGNED



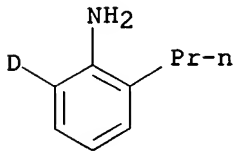
RN 1021325-42-7 CAPLUS
CN INDEX NAME NOT YET ASSIGNED



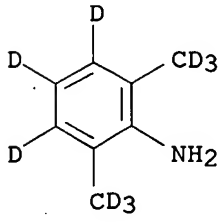
RN 1021325-43-8 CAPLUS
CN INDEX NAME NOT YET ASSIGNED



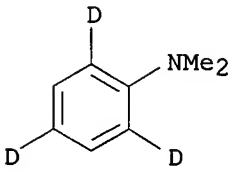
RN 1021325-44-9 CAPLUS
CN INDEX NAME NOT YET ASSIGNED



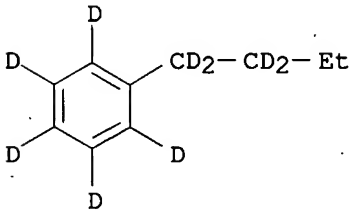
RN 1021325-45-0 CAPLUS
CN INDEX NAME NOT YET ASSIGNED



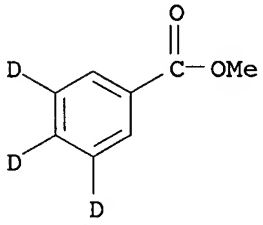
RN 1021325-46-1 CAPLUS
CN INDEX NAME NOT YET ASSIGNED



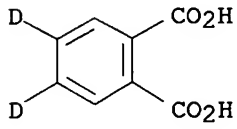
RN 1021325-47-2 CAPLUS
CN INDEX NAME NOT YET ASSIGNED



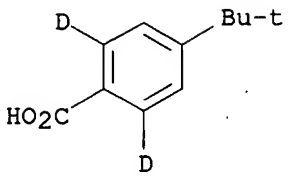
RN 1021325-48-3 CAPLUS
CN INDEX NAME NOT YET ASSIGNED



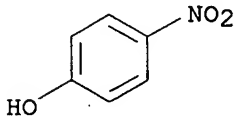
RN 1021325-49-4 CAPLUS
CN INDEX NAME NOT YET ASSIGNED



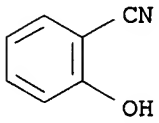
RN 1021325-50-7 CAPLUS
CN INDEX NAME NOT YET ASSIGNED



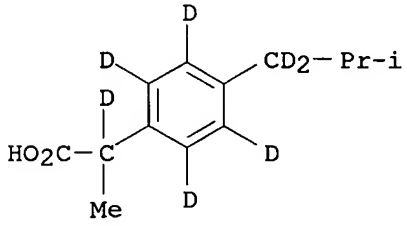

RN 1021325-51-8 CAPLUS
CN INDEX NAME NOT YET ASSIGNED




RN 1021325-52-9 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

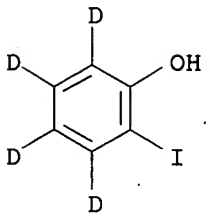



RN 1021325-53-0 CAPLUS
CN INDEX NAME NOT YET ASSIGNED




● Na

RN 1021325-54-1 CAPLUS
CN INDEX NAME NOT YET ASSIGNED




REFERENCE COUNT: 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 2 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2008:231428 CAPLUS
DOCUMENT NUMBER: 148:403501
TITLE: Histidine and deuterium labeled histidine by asymmetric catalytic reduction with gaseous H2 or D2; the role of strong non-coordinating acids
AUTHOR(S): Cesarotti, E.; Rimoldi, I.; Zerla, D.; Aldini, G.
CORPORATE SOURCE: Facolta di Farmacia, Dipartimento di Chimica Inorganica, Metallorganica e Analitica e Istituto CNR-ISTM, Universita di Milano, Milan, 20133, Italy
SOURCE: Tetrahedron: Asymmetry (2008), 19(3), 273-278
CODEN: TASYE3; ISSN: 0957-4166
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 148:403501

AB An efficient and convenient route for the preparation of natural and unnatural histidine by asym. hydrogenation with rhodium-phosphine complexes is described. The redns. were performed in the presence of HBF4 to generate an essential imidazolyl cation. Stereoselective incorporation of D2 in the α,β-positions was obtained by catalytic deuteration in the presence of MeOD.

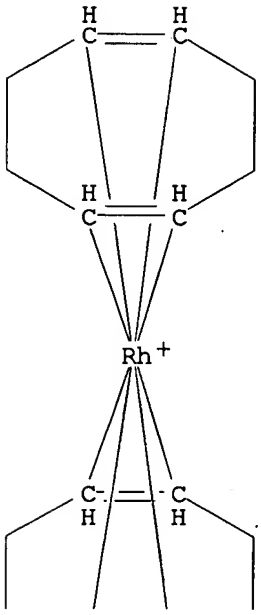
IT 59420-05-2, Bis(1,5-cyclooctadiene)rhodium perchlorate
RL: CAT (Catalyst use); USES (Uses)
(stereoselective preparation of histidine and deuterium labeled histidine and phenylalanine via rhodium-diphosphine-catalyzed asym. hydrogenation or deuteration of imidazolylpropenoate or phenyl(amido)propenoate)

RN 59420-05-2 CAPLUS
CN Rhodium(1+), bis[(1,2,5,6-η)-1,5-cyclooctadiene]-, perchlorate (1:1) (CA INDEX NAME)

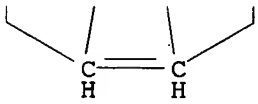
CM 1

CRN 35015-47-5
CMF C16 H24 Rh
CCI CCS

PAGE 1-A

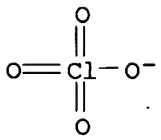


PAGE 2-A



CM 2

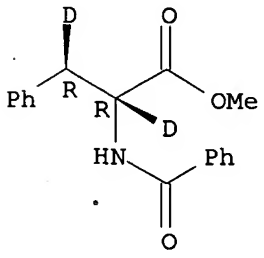
CRN 14797-73-0
CMF Cl O4



IT 95250-96-7P 1015244-10-6P 1015244-11-7P
1015478-57-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(stereoselective preparation of histidine and deuterium labeled histidine and phenylalanine via rhodium-diphosphine-catalyzed asym. hydrogenation or deuteration of imidazolylpropenoate or phenyl(amido)propenoate)
RN 95250-96-7 CAPLUS

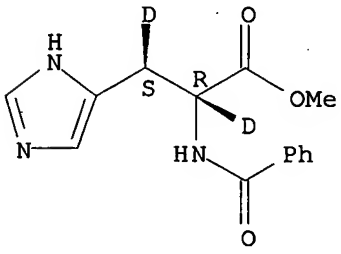
CN D-Phenylalanine-α,β-d2, N-benzoyl-, methyl ester, (βR)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



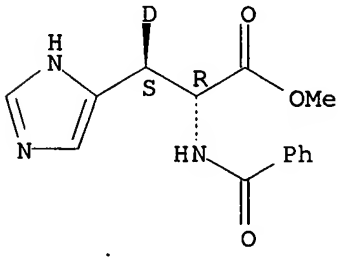
RN 1015244-10-6 CAPLUS
CN D-Histidine-α,β-d2, N-benzoyl-, methyl ester, (βS)- (CA INDEX NAME)

Absolute stereochemistry.



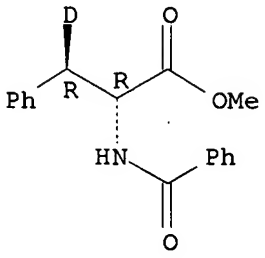
RN 1015244-11-7 CAPLUS
CN D-Histidine-β-d, N-benzoyl-, methyl ester, (βS)- (CA INDEX NAME)

Absolute stereochemistry.



RN 1015478-57-5 CAPLUS
CN D-Phenylalanine-β-d, N-benzoyl-, methyl ester, (βR)- (CA INDEX NAME)

Absolute stereochemistry.

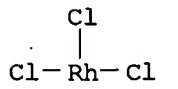


REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

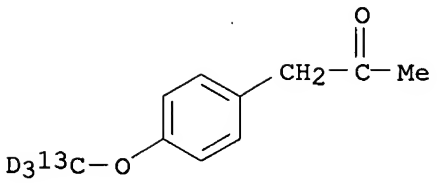
L24 ANSWER 3 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:1003752 CAPLUS
DOCUMENT NUMBER: 148:585188
TITLE: H/D-exchange reactions with hydride-activated catalysts
AUTHOR(S): Derdau, Volker; Atzrodt, Jens; Holla, Wolfgang
CORPORATE SOURCE: GMPK, Isotope Chemistry and Metabolite Synthesis Frankfurt, Sanofi-Aventis Deutschland GmbH, Frankfurt/Hoechst, 65926, Germany
SOURCE: Journal of Labelled Compounds and Radiopharmaceuticals (2007), 50(5-6), 295-299
CODEN: JLCRD4; ISSN: 0362-4803
PUBLISHER: John Wiley & Sons Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A safe, user friendly and efficient method to provide high D incorporation into a variety of organic substrates was developed. Systematic screening of catalysts and activators revealed that the activation of the Pd- or Rh-catalyst by NaBD4 is essential for the H/D exchange. The feasibility was demonstrated by the successful application of this method to bi- and tricyclic aromatic compds. as well as chiral natural products like dextromethorphan or drugs like formoterol.

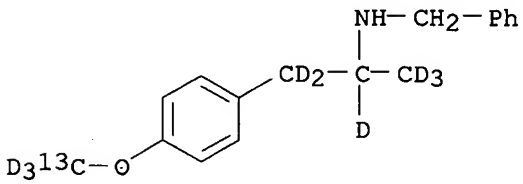
IT 10049-07-7, Rhodium chloride (RhCl3)
RL: CAT (Catalyst use); USES (Uses)
(H/D-exchange reactions with hydride-activated palladium and rhodium catalysts)
RN 10049-07-7 CAPLUS
CN Rhodium chloride (RhCl3) (CA INDEX NAME)



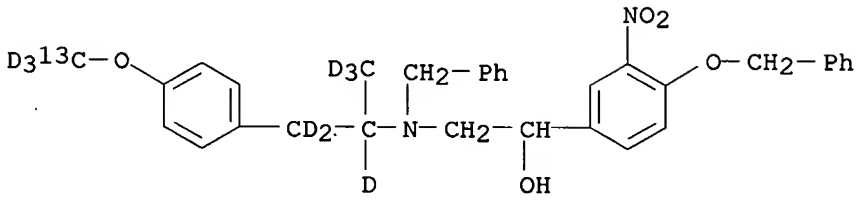
IT 1028681-09-5P 1028681-11-9P 1028681-14-2P
1028681-16-4P 1028681-26-6P 1028681-41-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(H/D-exchange reactions with hydride-activated palladium and rhodium catalysts)
RN 1028681-09-5 CAPLUS
CN INDEX NAME NOT YET ASSIGNED



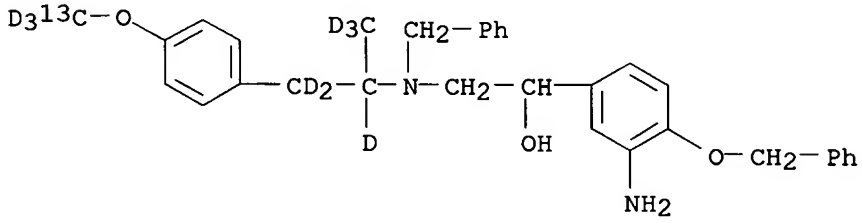
RN 1028681-11-9 CAPLUS
CN INDEX NAME NOT YET ASSIGNED



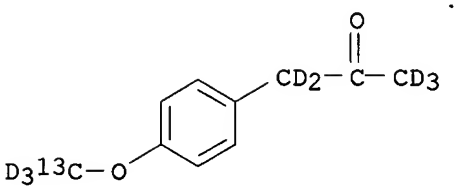
RN 1028681-14-2 CAPLUS
CN INDEX NAME NOT YET ASSIGNED



RN 1028681-16-4 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

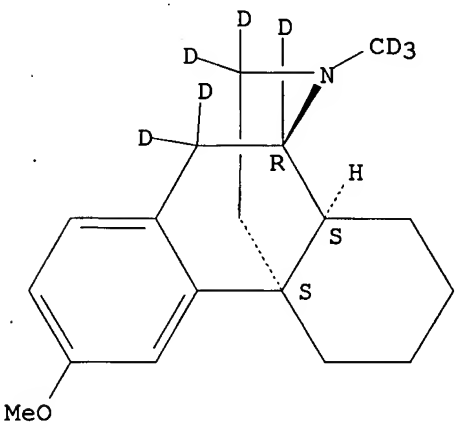


RN 1028681-26-6 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

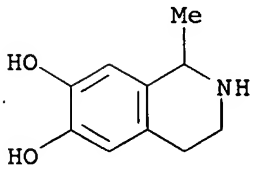


RN 1028681-41-5 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

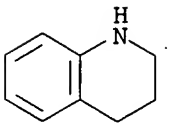
Absolute stereochemistry.



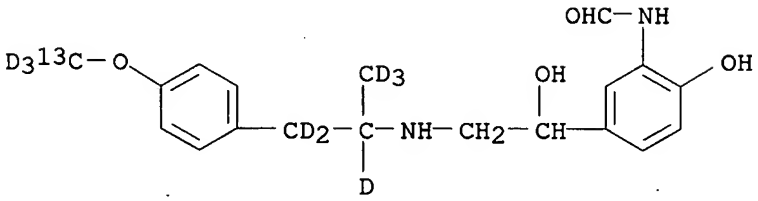
IT 915232-16-5P, 1,2,3,4-Tetrahydro-1-methylisoquinoline-6,7-diol labeled with deuterium 915232-18-7P, 1,2,3,4-Tetrahydroquinoline labeled with deuterium 1028681-18-6P 1028681-22-2P 1028681-24-4P 1028681-28-8P 1028681-31-3P, 2,2,3,3,4,4-Hexadeutero-1,2,3,4-tetrahydronaphthalen-1-one 1028681-35-7P 1028681-37-9P 1028681-39-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(H/D-exchange reactions with hydride-activated palladium and rhodium catalysts)
RN 915232-16-5 CAPLUS
CN 6,7-Isoquinolinediol, 1,2,3,4-tetrahydro-1-methyl-, labeled with deuterium (CA INDEX NAME)



RN 915232-18-7 CAPLUS
CN Quinoline, 1,2,3,4-tetrahydro-, labeled with deuterium (CA INDEX NAME)

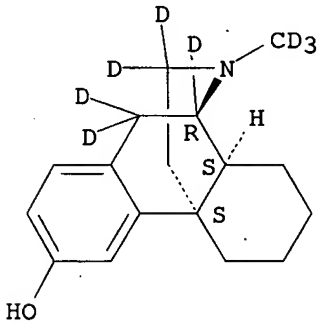


RN 1028681-18-6 CAPLUS
CN INDEX NAME NOT YET ASSIGNED



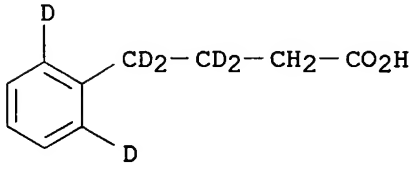
RN 1028681-22-2 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.



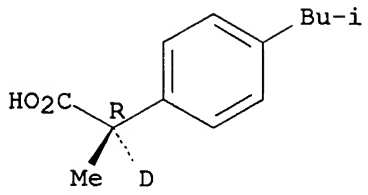
● HBr

RN 1028681-24-4 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

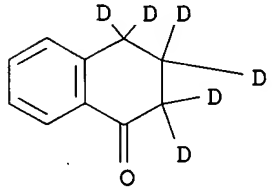


RN 1028681-28-8 CAPLUS
CN INDEX NAME NOT YET ASSIGNED

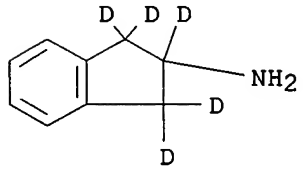
Absolute stereochemistry.



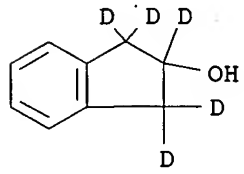

RN 1028681-31-3 CAPLUS
CN INDEX NAME NOT YET ASSIGNED



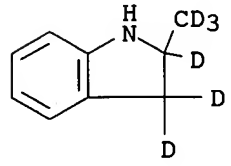

RN 1028681-35-7 CAPLUS
CN INDEX NAME NOT YET ASSIGNED




RN 1028681-37-9 CAPLUS
CN INDEX NAME NOT YET ASSIGNED




RN 1028681-39-1 CAPLUS
CN INDEX NAME NOT YET ASSIGNED



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 4 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:908108 CAPLUS
DOCUMENT NUMBER: 147:406255
TITLE: C-H bond activation by water on a palladium or platinum metal surface
AUTHOR(S): Matsubara, Seijiro; Asano, Keisuke; Kajita, Yuichi; Yamamoto, Mitsuru
CORPORATE SOURCE: Department of Material Chemistry, Graduate School of Engineering, Kyoto University, Kyoudai-katsura, Kyoto, 606-8501, Japan
SOURCE: Synthesis (2007), (13), 2055-2059
CODEN: SYNTBF; ISSN: 0039-7881
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 147:406255
AB A water mol. is partially cleaved on a palladium or platinum metal surface under hydrothermal conditions to form an active platinum species. The species is effective for C-H bond functionalization which can be applied for H/D-exchange reactions, C-C bond-forming reactions, and C-N bond-forming reactions.
IT 1314-15-4, Platinum oxide (PtO2) 7440-06-4, Platinum, uses 7718-54-9, Nickel chloride, uses
RL: CAT (Catalyst use); USES (Uses)
(C-H bond activation by water on a palladium or platinum metal surface)
RN 1314-15-4 CAPLUS
CN Platinum oxide (PtO2) (CA INDEX NAME)

O=Pt=O

RN 7440-06-4 CAPLUS
CN Platinum (CA INDEX NAME)

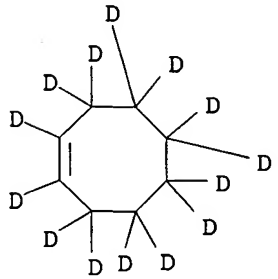
Pt

RN 7718-54-9 CAPLUS
CN Nickel chloride (NiCl2) (CA INDEX NAME)

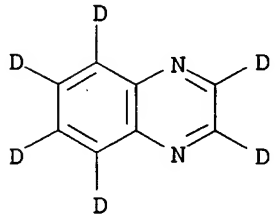
Cl-Ni-Cl

IT 10249-89-5P 20617-93-0P, Quinoxaline-2,3,5,6,7,8-d6
32190-42-4P 34071-94-8P, Quinoline-2,3,4,5,6,7,8-d7
73509-20-3P, 1H-Indole-1,2,3,4,5,6,7-d7 97797-70-1P
97960-58-2P 132125-39-4P 634897-78-2P
880462-22-6P 951164-40-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(C-H bond activation by water on a palladium or platinum metal surface)
RN 10249-89-5 CAPLUS

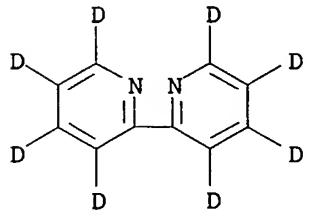
CN Cyclooctene-1,2,3,3,4,4,5,5,6,6,7,7,8,8-d14 (CA INDEX NAME)



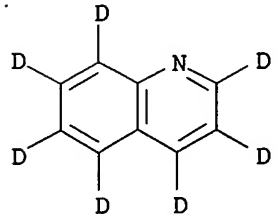
RN 20617-93-0 CAPLUS
CN Quinoxaline-2,3,5,6,7,8-d6 (CA INDEX NAME)



RN 32190-42-4 CAPLUS
CN 2,2'-Bipyridine-3,3',4,4',5,5',6,6'-d8 (CA INDEX NAME)

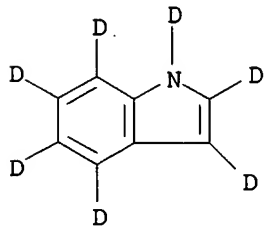


RN 34071-94-8 CAPLUS
CN Quinoline-2,3,4,5,6,7,8-d7 (CA INDEX NAME)



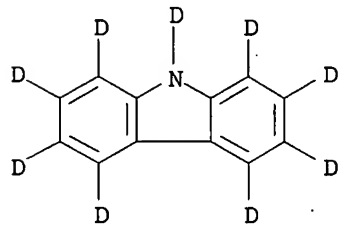
RN 73509-20-3 CAPLUS

CN 1H-Indole-1,2,3,4,5,6,7-d7 (CA INDEX NAME)

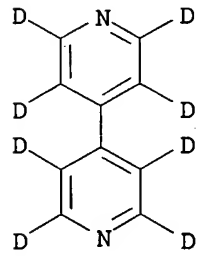


RN 97797-70-1 CAPLUS
CN Cyclododecene-1,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,12,12-d22 (CA INDEX NAME)

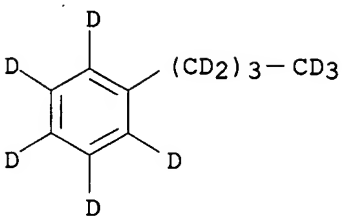
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
RN 97960-58-2 CAPLUS
CN 9H-Carbazole-1,2,3,4,5,6,7,8,9-d9 (CA INDEX NAME)



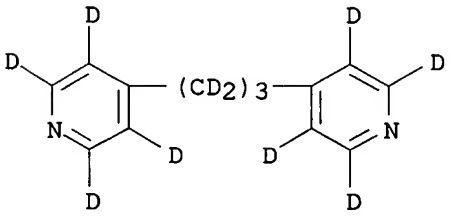
RN 132125-39-4 CAPLUS
CN 4,4'-Bipyridine-2,2',3,3',5,5',6,6'-d8 (CA INDEX NAME)



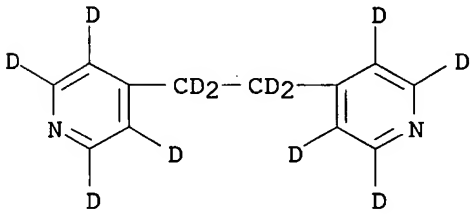
RN 634897-78-2 CAPLUS
CN Benzene-1,2,3,4,5-d5, 6-(butyl-1,1,2,2,3,3,4,4,4-d9)- (CA INDEX NAME)



RN 880462-22-6 CAPLUS
CN Pyridine-2,3,5,6-d4, 4,4'-(1,3-propanediyl-1,1,2,2,3,3-d6)bis- (CA INDEX NAME)



RN 951164-40-2 CAPLUS
CN Pyridine-2,3,5,6-d4, 4,4'-(1,2-ethanediyl-1,1,2,2-d4)bis- (CA INDEX NAME)



IT 7440-02-0, Raney nickel, uses
RL: CAT (Catalyst use); USES (Uses)
(catalysts; C-H bond activation by water on a palladium or platinum metal surface)
RN 7440-02-0 CAPLUS
CN Nickel (CA INDEX NAME)

Ni

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 5 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:589355 CAPLUS
DOCUMENT NUMBER: 147:9672
TITLE: Procedure for the catalytic deuteration of organic

compounds
PATENT ASSIGNEE(S): Sanofi-Aventis Deutschland G.m.b.H., Germany
SOURCE: Ger. Offen., 4pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| DE 102005056856 | A1 | 20070531 | DE 2005-102005056856 | 20051128 |
| PRIORITY APPLN. INFO.: | | | DE 2005-102005056856 | 20051128 |

OTHER SOURCE(S): CASREACT 147:9672

AB The deuteration of organic compds. (e.g., phenylbutyric acid) is achieved by suspending the compound in D2O, adding transition metal catalyst (e.g., 10% Pd/C), followed by the addition of at least a deuteride (e.g., NaBD4) and/or a hydride.

IT 7440-06-4, Platinum, uses 7440-16-6, Rhodium, uses
RL: CAT (Catalyst use); USES (Uses)
(in a procedure for the catalytic deuteration of organic compds.)

RN 7440-06-4 CAPLUS
CN Platinum (CA INDEX NAME)

Pt

RN 7440-16-6 CAPLUS
CN Rhodium (CA INDEX NAME)

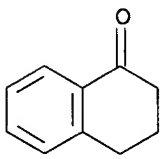
Rh

IT 651316-73-3P 915232-14-3P 915232-20-1P
915232-22-3P 915232-24-5P 915232-26-7P
937737-31-0P 937737-32-1P 937737-33-2P
937737-34-3P, preparation 937737-35-4P
937803-10-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(procedure for the catalytic deuteration of organic compds.)

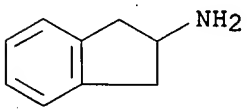
RN 651316-73-3 CAPLUS
CN Benzenebutanoic acid, labeled with deuterium (CA INDEX NAME)

$HO_2C-(CH_2)_3-Ph$

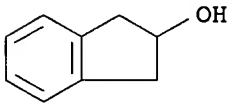
RN 915232-14-3 CAPLUS
CN 1(2H)-Naphthalenone, 3,4-dihydro-, labeled with deuterium (CA INDEX NAME)



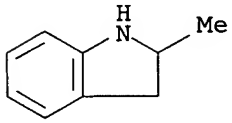
RN 915232-20-1 CAPLUS
CN 1H-Inden-2-amine, 2,3-dihydro-, labeled with deuterium (CA INDEX NAME)



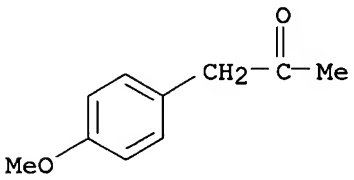
RN 915232-22-3 CAPLUS
CN 1H-Inden-2-ol, 2,3-dihydro-, labeled with deuterium (CA INDEX NAME)



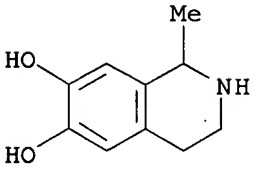
RN 915232-24-5 CAPLUS
CN 1H-Indole, 2,3-dihydro-2-methyl-, labeled with deuterium (CA INDEX NAME)



RN 915232-26-7 CAPLUS
CN 2-Propanone, 1-(4-methoxyphenyl)-, labeled with deuterium (CA INDEX NAME)

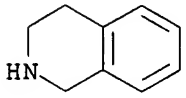


RN 937737-31-0 CAPLUS
CN 6,7-Isoquinolinediol, 1,2,3,4-tetrahydro-1-methyl-, labeled with deuterium, hydrochloride (1:1) (CA INDEX NAME)

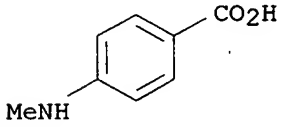


● HCl

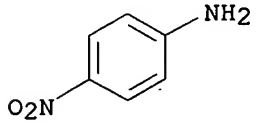
RN 937737-32-1 CAPLUS
CN Isoquinoline, 1,2,3,4-tetrahydro-, labeled with deuterium (CA INDEX NAME)



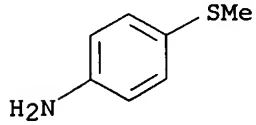
RN 937737-33-2 CAPLUS
CN Benzoic acid, 4-(methylamino)-, labeled with deuterium (9CI) (CA INDEX NAME)



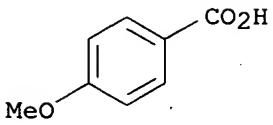
RN 937737-34-3 CAPLUS
CN Benzenamine, 4-nitro-, labeled with deuterium (9CI) (CA INDEX NAME)



RN 937737-35-4 CAPLUS
CN Benzenamine, 4-(methylthio)-, labeled with deuterium (9CI) (CA INDEX NAME)



RN 937803-10-6 CAPLUS
CN Benzoic acid, 4-methoxy-, labeled with deuterium (CA INDEX NAME)




REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 6 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:477634 CAPLUS
DOCUMENT NUMBER: 147:118292
TITLE: Rhodium- and Iridium-Catalyzed Double Hydroalkoxylation of Alkynes, an Efficient Method for the Synthesis of O,O-Acetals: Catalytic and Mechanistic Studies
AUTHOR(S): Messerle, Barbara A.; Vuong, Khuong Q.
CORPORATE SOURCE: School of Chemistry, University of New South Wales, Kensington, NSW 2052, Australia
SOURCE: Organometallics (2007), 26(12), 3031-3040
CODEN: ORGND7; ISSN: 0276-7333
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 147:118292

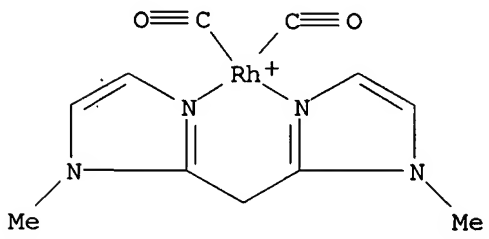
AB An efficient method for the synthesis of O,O-acetals via metal-catalyzed double hydroalkoxylation of alkynes was developed using the Ir(I) and Rh(I) complexes [Ir(PyP)(CO)2]BPh4 (1) and [Rh(bim)(CO)2]BPh4 (2), where PyP = 1-[2-(diphenylphosphino)ethyl]pyrazole and bim = bis(N-methylimidazol-2-yl)methane, as catalysts for the consecutive addition of two alc. functional groups to terminal and nonterminal alkynes to form O,O-acetals. When the catalyzed cyclization of alkynols was performed in the presence of an excess amount of MeOH as a cosolvent, a mol. of MeOH was incorporated into the acetal product. The catalyzed cyclization of alkynols in the absence of an alc. solvent led to cyclization with incorporation of a 2nd mol. of substrate in the final acetal product. Complexes 1 and 2 were also effective as catalysts for the cyclization of alkyne diols to form bicyclic O,O-acetals. The Ir complex 1 was more efficient than the Rh complex 2 in promoting the reactions of aliphatic alkyne diols. However, the Rh complex 2 was more effective for promoting the reactions of aromatic substrates. Mechanistic study using low-temperature NMR spectroscopy showed that the catalytic cycle proceeded via π coordination of the alkyne of the substrate to the metal center followed by the sequential addition of two hydroxyl groups to form O,O-acetals. Deuteration studies and anal. of reaction intermediates supported the proposed mechanism.

IT 251441-52-8
RL: CAT (Catalyst use); USES (Uses)
(rhodium- and iridium-catalyzed double hydroalkoxylation of alkynols and alkyne diols to give cyclic and bicyclic acetals, resp.)

RN 251441-52-8 CAPLUS
CN Rhodium(1+), dicarbonyl[2,2'-methylenebis[1-methyl-1H-imidazole-κN3]]-, (SP-4-2)-, tetraphenylborate(1-) (9CI) (CA INDEX NAME)

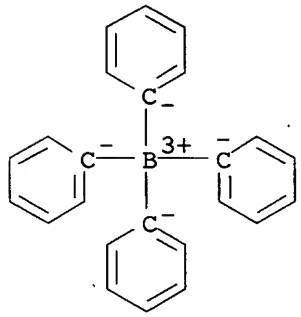
CM 1

CRN 251441-51-7
CMF C11 H12 N4 O2 Rh
CCI CCS



CM 2

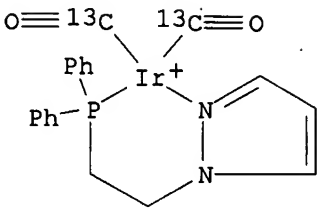
CRN 4358-26-3
CMF C24 H20 B
CCI CCS



IT 935764-78-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(rhodium- and iridium-catalyzed double hydroalkoxylation of alkynols and alkyne diols to give cyclic and bicyclic acetals, resp.)
RN 935764-78-6 CAPLUS
CN Iridium(1+), di(carbonyl-13C)[1-[2-(diphenylphosphino-κP)ethyl]-1H-pyrazole-κN2]-, (SP-4-3)-, tetraphenylborate(1-) (1:1) (CA INDEX NAME)

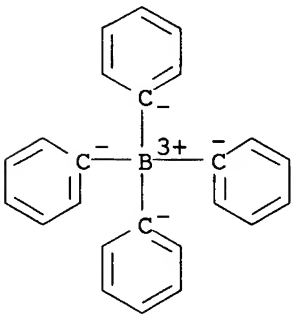
CM 1

CRN 935764-77-5
CMF C19 H17 Ir N2 O2 P
CCI CCS



CM 2

CRN 4358-26-3
CMF C24 H20 B
CCI CCS

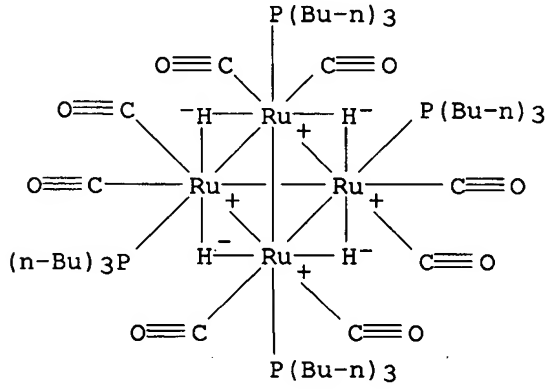


REFERENCE COUNT: 67 THERE ARE 67 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 7 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:444165 CAPLUS
DOCUMENT NUMBER: 147:72560
TITLE: A Convenient Route to the Synthesis of Isotopomeric Dihydro-2(3H)furanones
AUTHOR(S): Frediani, Piero; Rosi, Luca; Frediani, Marco; Bartolucci, Gianluca; Bambagiotti-Alberti, Massimo
CORPORATE SOURCE: Department of Organic Chemistry, University of Florence, Florence, 13-50019, Italy
SOURCE: Journal of Agricultural and Food Chemistry (2007), 55(10), 3877-3883
CODEN: JAFCAU; ISSN: 0021-8561
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 147:72560
AB A general synthetic procedure leading to isotopomeric dihydro-2(3H)furanones (γ-butyrolactones) containing two, four, or six deuterium atoms has been developed. The labeled dihydro-2(3H)furanones were synthesized in quant. yield from the saturated diacid C4 (succinic) or unsatd. diacids C4 (fumaric, maleic, or acetylenedicarboxylic) in the presence of Ru4H4(CO)8(PBu3)4 using a deuterium pressure of 180 bar at 180 °C. This methodol. was applied to the total synthesis of a hexadeuterated matairesinol lignan: The 3,4-bis{[3-methoxy-4-

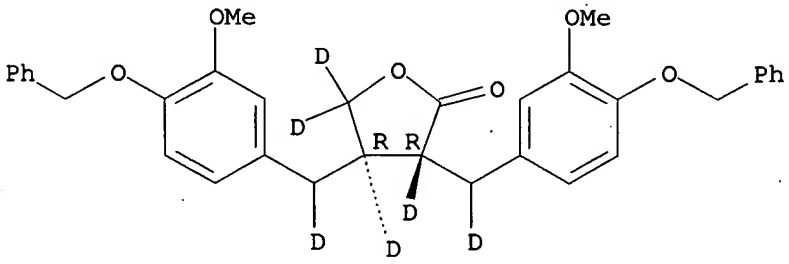
(phenylmethoxy)phenyl]methyl)dihydro-2(3H)furanone-[7,7',8,8',9,9'-D6] (benzyl-protected matairesinol-D6) was fully characterized.

IT 34742-78-4
RL: CAT (Catalyst use); USES (Uses)
(preparation of dihydrofuranones via ring-closing deuteration)
RN 34742-78-4 CAPLUS
CN Ruthenium, octacarbonyltetra-μ-hydrotetrakis(tributylphosphine)tetra-, tetrahedro (9CI) (CA INDEX NAME)



IT 941307-25-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of matairesinol-D6 derivative via ring-closing deuteration)
RN 941307-25-1 CAPLUS
CN 2(3H)-Furanone-3,4,5-d3, dihydro-5-d-3,4-bis[[3-methoxy-4-(phenylmethoxy)phenyl]methyl-d]-, (3R,4R)-rel- (CA INDEX NAME)

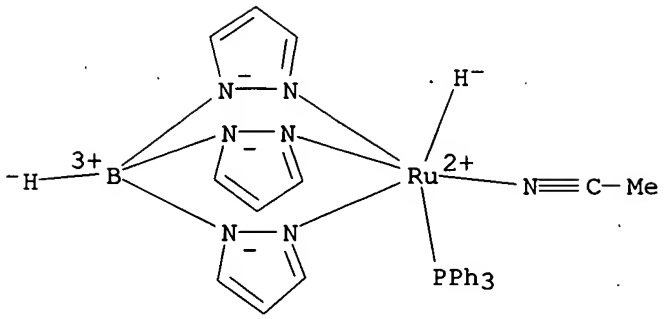
Relative stereochemistry.



REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

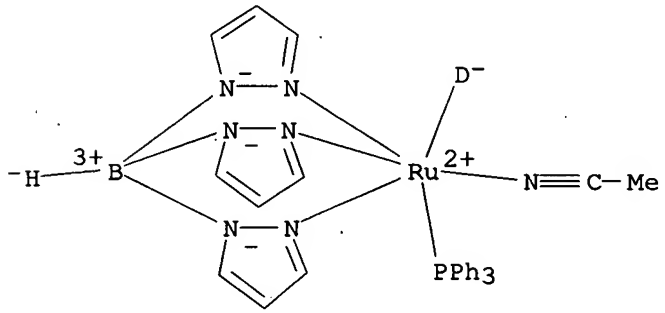
L24 ANSWER 8 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:269690 CAPLUS
DOCUMENT NUMBER: 146:482144
TITLE: Catalytic H/D Exchange between Organic Compounds and D2O with TpRu(PPh3)(CH3CN)H (Tp = hydro(trispyrazolyl)borate). Reaction of TpRu(PPh3)(CH3CN)H with Water to Form Acetamido Complex TpRu(PPh3)(H2O)(NHC(O)CH3)
AUTHOR(S): Leung, Chung Wing; Zheng, Wenxu; Wang, Dexian; Ng, Siu

Man; Yeung, Chi Hung; Zhou, Zhongyuan; Lin, Zhenyang; Lau, Chak Po
CORPORATE SOURCE: Department of Applied Biology and Chemical Technology, The Hong Kong Polytechnic University, Hung Hom, Kowloon, Hong Kong, Peop. Rep. China
SOURCE: Organometallics (2007), 26(8), 1924-1933
CODEN: ORGND7; ISSN: 0276-7333
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 146:482144
AB Deuteration of organic mols. using D2O as the D source is affected with catalytic systems based on the Ru solvento hydride complex TpRu(PPh3)(MeCN)H. The deuteration reactions can be performed under Ar or H2. In the former case, the hydride ligand is rapidly deuterated by D2O, and in the catalysis, D2O converts TpRu(PPh3)(MeCN)D into the acetamido complex TpRu(PPh3)(D2O)(NDC(O)CH3), which at the later stage of the reaction generates two addnl. minor species, one of which is the partially deuterated carbonyl hydride species TpRu(PPh3)(CO)H(or D). All of these complexes are, however, found to be inactive for the H/D exchange reactions between the organic mols. and D2O. In the exchange reactions under H2, a mixture of the HD isotopomers, TpRu(PPh3)H3-xDx, of the dihydrogen hydride complex TpRu(PPh3)(H2)H are the active species. The solvento complex TpRu(PPh3)(MeCN)D under Ar probably is more active than TpRu(PPh3)(H3-x)Dx under H2 for the H/D exchange reactions because the former reacts more readily with the organic mol. R-H to generate the η2-R-H σ-complex due to higher lability of the MeCN ligand in comparison with the dihydrogen or H-D ligand of TpRu(PPh3)(H3-x)Dx. The acetamido complex TpRu(PPh3)(H2O)(NHC(O)CH3) was independently prepared by refluxing a THF solution of TpRu(PPh3)(MeCN)H containing excess H2O for 24 h, and its mol. structure was determined by x-ray crystallog. Theor. calcns. at the Becke3LYP level of DFT theory were performed to study the reaction of TpRu(PPh3)(MeCN)H with H2O that leads to the formation TpRu(PPh3)(H2O)(NHC(O)CH3). The hydration reaction is promoted by a Ru-H···H-OH dihydrogen-bonding interaction between the hydride ligand and the attacking H2O mol. An explanation for the failure of the chloro analog TpRu(PPh3)(MeCN)Cl to react with H2O to form the acetamido complex is also provided.
IT 185221-92-5
RL: CAT (Catalyst use); RCT (Reactant); RACT (Reactant or reagent); USES (Uses)
(hydrolysis of (hydrotrispyrazolylborato)(hydrido)ruthenium acetonitrile to give an acetamido complex and catalytic activity for H/D exchange between organic compds. and dideuterium oxide)
RN 185221-92-5 CAPLUS
CN Ruthenium, (acetonitrile)hydro[hydrotris(1H-pyrazolato-κN1)borato(1-)-κN2,κN2',κN2'']( triphenylphosphine)-, (OC-6-24)- (9CI) (CA INDEX NAME)

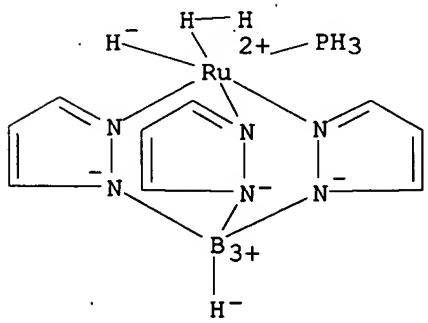


IT 540729-60-0P 936010-53-6P 936010-54-7P
936010-55-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(hydrolysis of (hydrotrispyrazolylborato)(hydrido)ruthenium acetonitrile to give an acetamido complex and catalytic activity for H/D exchange between organic compds. and dideuterium oxide)

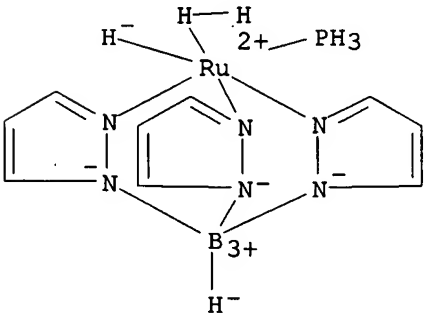
RN 540729-60-0 CAPLUS
CN Ruthenium, (acetonitrile)hydro-d-[hydrotris(1H-pyrazolato-κN1)borato(1-)-κN2,κN2',κN2''](triphenylphosphine)-, (OC-6-24)- (9CI) (CA INDEX NAME)



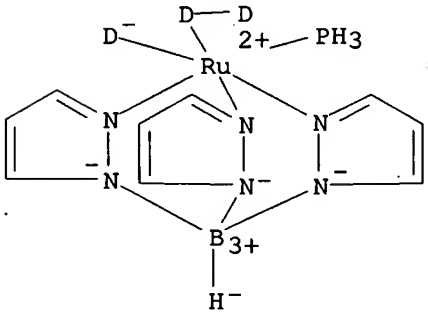
RN 936010-53-6 CAPLUS
CN Ruthenium, (dihydrogen-κH1,κH2)hydro[hydrotris(1H-pyrazolato-κN1)borato(1-)-κN2,κN2',κN2'']phosphine)-, labeled with deuterium (CA INDEX NAME)



RN 936010-54-7 CAPLUS
CN Ruthenium, (dihydrogen-κH1,κH2)hydro[hydrotris(1H-pyrazolato-κN1)borato(1-)-κN2,κN2',κN2'']phosphine)-, labeled with deuterium (CA INDEX NAME)



RN 936010-55-8 CAPLUS
CN Ruthenium, (dihydrogen-d2-κD1,κD2)hydro-d-[hydrotris(1H-pyrazolato-κN1)borato(1-)-κN2,κN2',κN2'']phosphine)- (CA INDEX NAME)



REFERENCE COUNT: 61 THERE ARE 61 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 9 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:199776 CAPLUS
DOCUMENT NUMBER: 146:421550
TITLE: Mechanistic study of a Pd/C-catalyzed reduction of aryl sulfonates using the Mg-MeOH-NH4OAc system
AUTHOR(S): Mori, Akinori; Mizusaki, Tomoteru; Ikawa, Takashi; Maegawa, Tomohiro; Monguchi, Yasunari; Sajiki, Hironao
CORPORATE SOURCE: Laboratory of Medicinal Chemistry, Gifu Pharmaceutical University, Mitahora-higashi 5-6-1, Gifu, 8585, Japan
SOURCE: Chemistry--A European Journal (2007), 13(5), 1432-1441
CODEN: CEUJED; ISSN: 0947-6539
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 146:421550
AB A method for the deoxygenation of phenolic hydroxy groups via aryl triflates or mesylates has been established by using a combination of

Pd/C-Mg-MeOH. The addition of NH4OAc to the system markedly accelerated the reaction rate and expanded the scope of the reaction. Mechanistic studies suggested that a single-electron transfer process from the Pd0 center to the benzene ring is involved in the reduction of aryl sulfonates and that NH4OAc works as a solubilization reagent of the Mg salt and as an accelerator of the electron transfer, thus enhancing the reaction process. Our method was also applicable to the regioselective deuteration of benzene derivs. with CH3OD as the solvent and deuterium source: the original hydroxy group could be efficiently replaced with a deuterium atom.

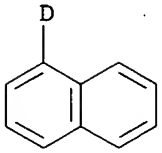
IT 7440-02-0, Nickel, uses
RL: CAT (Catalyst use); PEP (Physical, engineering or chemical process); PROC (Process); USES (Uses)
(mechanistic study of Pd/C-catalyzed reduction of aryl sulfonates using Mg-MeOH-NH4OAc system)

RN 7440-02-0 CAPLUS
CN Nickel (CA INDEX NAME)

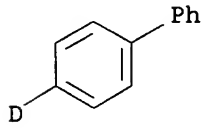
Ni

IT 875-62-7P, Naphthalene-1-d 4819-98-1P, 1,1'-Biphenyl-4-d
87449-73-8P 934176-12-2P 934176-13-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(mechanistic study of Pd/C-catalyzed reduction of aryl sulfonates using Mg-MeOH-NH4OAc system)

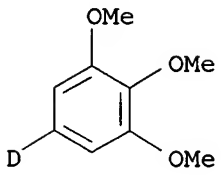
RN 875-62-7 CAPLUS
CN Naphthalene-1-d (CA INDEX NAME)



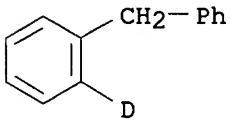

RN 4819-98-1 CAPLUS
CN 1,1'-Biphenyl-4-d (CA INDEX NAME)



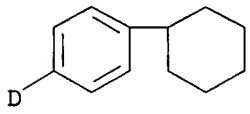

RN 87449-73-8 CAPLUS
CN Benzene-d, 3,4,5-trimethoxy- (CA INDEX NAME)




RN 934176-12-2 CAPLUS
CN Benzene-d, 2-(phenylmethyl)- (CA INDEX NAME)




RN 934176-13-3 CAPLUS
CN Benzene-d, 4-cyclohexyl- (CA INDEX NAME)



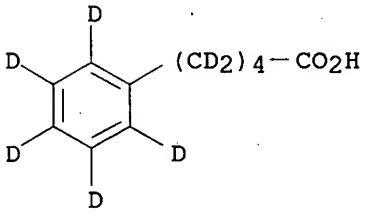

REFERENCE COUNT: 57 THERE ARE 57 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 10 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:689620 CAPLUS
DOCUMENT NUMBER: 146:421688
TITLE: Synergistic effect of a palladium-on-carbon/platinum-on-carbon mixed catalyst in hydrogen/deuterium exchange reactions of alkyl-substituted aromatic compounds
AUTHOR(S): Ito, Nobuhiro; Watahiki, Tsutomu; Maesawa, Tsuneaki; Maegawa, Tomohiro; Sajiki, Hironao
CORPORATE SOURCE: Chemical Products Research Laboratories, Wako Pure Chemical Industries, Ltd., 1633 Matoba, Kawagoe, 350-1101, Japan
SOURCE: Advanced Synthesis & Catalysis (2006), 348(9), 1025-1028
CODEN: ASCAF7; ISSN: 1615-4150
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A synergistic effect in the H-D exchange reaction of alkyl-substituted aromatic compds. using the Pd/C-Pt/C-D2O-H2 system was discovered. This system would lead to fully H-D exchange results even on the sterically hindered sites which were only low-deuterium incorporated by Pd/C or Pt/C independently. Since the reaction was general for a variety of aromatic compds., it could be applied to the deuteration of dianiline derivs. as raw materials for polyimides.
IT 7440-06-4, Platinum, uses

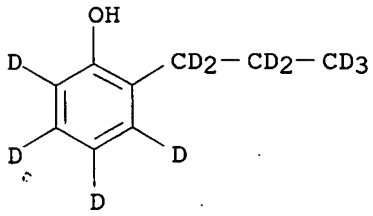
RL: CAT (Catalyst use); USES (Uses)
(synergistic effect of palladium-on-carbon/platinum-on-carbon mixed catalyst in hydrogen/deuterium exchange reaction of alkyl-substituted aromatic compds.)
RN 7440-06-4 CAPLUS
CN Platinum (CA INDEX NAME)

Pt

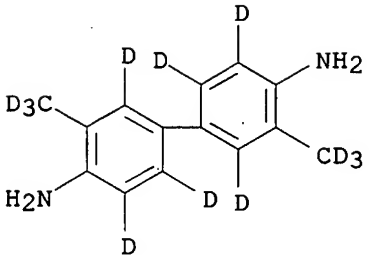
IT 767627-97-4P, Benzene-d5-pentanoic-d8 acid 861405-62-1P
870284-54-1P 870284-60-9P 870284-63-2P
870284-66-5P 870284-69-8P 934266-51-0P
934266-52-1P 934266-54-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synergistic effect of palladium-on-carbon/platinum-on-carbon mixed catalyst in hydrogen/deuterium exchange reaction of alkyl-substituted aromatic compds.)
RN 767627-97-4 CAPLUS
CN Benzene-d5-pentanoic-d8 acid (CA INDEX NAME)



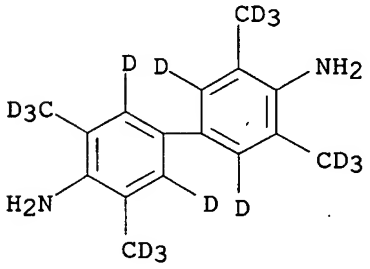

RN 861405-62-1 CAPLUS
CN Phen-2,3,4,5-d4-ol, 6-(propyl-d7)- (CA INDEX NAME)



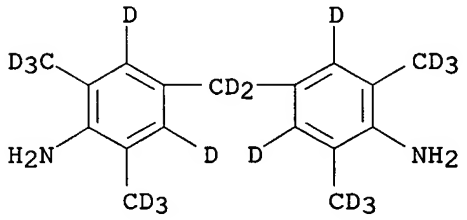

RN 870284-54-1 CAPLUS
CN [1,1'-Biphenyl-2,2',3,3',6,6'-d6]-4,4'-diamine, 5,5'-di(methyl-d3)- (CA INDEX NAME)



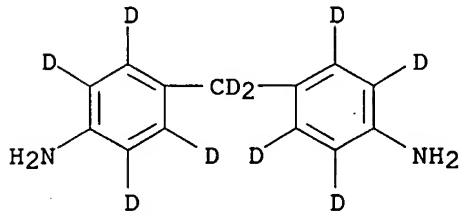
RN 870284-60-9 CAPLUS
CN [1,1'-Biphenyl-2,2',6,6'-d4]-4,4'-diamine, 3,3',5,5'-tetra(methyl-d3)- (9CI) (CA INDEX NAME)



RN 870284-63-2 CAPLUS
CN Benzen-3,5-d2-amine, 4,4'-(methylene-d2)bis[2,6-di(methyl-d3)- (CA INDEX NAME)

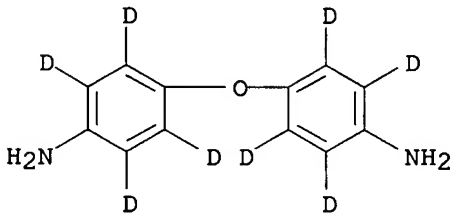


RN 870284-66-5 CAPLUS
CN Benzen-2,3,5,6-d4-amine, 4,4'-(methylene-d2)bis- (CA INDEX NAME)

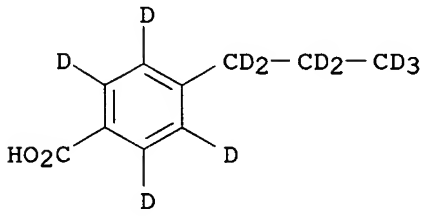


RN 870284-69-8 CAPLUS

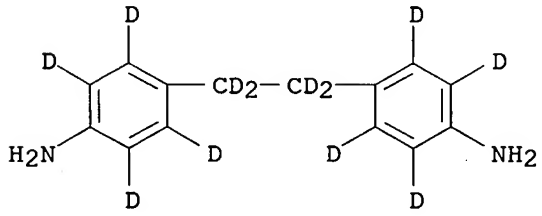
CN Benzen-2,3,5,6-d4-amine, 4,4'-oxybis- (CA INDEX NAME)



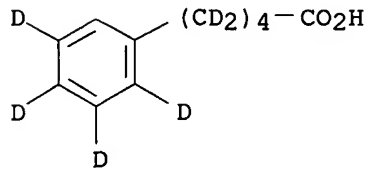
RN 934266-51-0 CAPLUS
CN Benzoic-2,3,5,6-d4 acid, 4-(propyl-1,1,2,2,3,3,3-d7)- (CA INDEX NAME)



RN 934266-52-1 CAPLUS
CN Benzen-2,3,5,6-d4-amine, 4,4'-(1,2-ethanediyl-1,1,2,2-d4)bis- (CA INDEX NAME)



RN 934266-54-3 CAPLUS
CN Benzene-2,3,4,5-d4-pentanoic-α,α,β,β,γ,γ,δ,δ-d8 acid (CA INDEX NAME)



REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

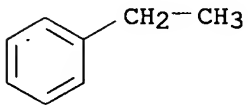
L24 ANSWER 11 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:559644 CAPLUS
DOCUMENT NUMBER: 145:166763
TITLE: Microwave-assisted reduction of acetophenones using Ni-Al alloy in water
AUTHOR(S): Miyazawa, Akira; Tashiro, Masashi; Prakash, G. K. Surya; Olah, George A.
CORPORATE SOURCE: National Institute of Advanced Industrial Science and Technology (AIST), 1-1-1 Higashi, Tsukuba, 305-8565, Japan
SOURCE: Bulletin of the Chemical Society of Japan (2006), 79(5), 791-792
CODEN: BCSJA8; ISSN: 0009-2673
PUBLISHER: Chemical Society of Japan
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 145:166763

AB The reduction of acetophenones using a Ni-Al alloy catalyst in water (H2O and D2O) under microwave irradiation proceeded to give the corresponding (deuterated) alkylbenzenes in good yields.

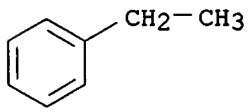
IT 11114-68-4
RL: CAT (Catalyst use); RCT (Reactant); RACT (Reactant or reagent); USES (Uses)
(Raney alloy; microwave-assisted reduction of acetophenones using Ni-Al alloy in water)
RN 11114-68-4 CAPLUS
CN Aluminum alloy, nonbase, Al,Ni (CA INDEX NAME)

| Component | Component Registry Number |
|---|---|
| Al | 7429-90-5 |
| Ni | 7440-02-0 |

IT 182579-04-0P, Ethylbenzene-d5, preparation 182579-06-2P, Ethylbenzene-d7, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(microwave-assisted reduction of acetophenones using Ni-Al alloy in water)
RN 182579-04-0 CAPLUS
CN Benzene, ethyl-, labeled with deuterium (9CI) (CA INDEX NAME)



RN 182579-06-2 CAPLUS
CN Benzene, ethyl-, labeled with deuterium (9CI) (CA INDEX NAME)

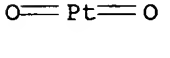


REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

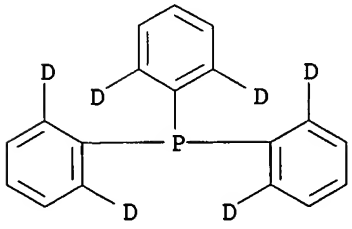
L24 ANSWER 12 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:93399 CAPLUS
DOCUMENT NUMBER: 144:330848
TITLE: Platinum catalyzed H-D exchange reaction of various aromatic compounds under hydrothermal condition
AUTHOR(S): Yamamoto, Mitsuru; Oshima, Koichiro; Matsubara, Seijiro
CORPORATE SOURCE: Department of Material Chemistry, Graduate School of Engineering, Kyoto University, Kyoudai-katsura, Nishikyo, Kyoto, 615-8510, Japan
SOURCE: Heterocycles (2006), 67(1), 353-359
CODEN: HTCYAM; ISSN: 0385-5414
PUBLISHER: Japan Institute of Heterocyclic Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:330848

AB Various aromatic compds. were treated with deuterium oxide under hydrothermal conditions in the presence of a catalytic amount of platinum(IV) oxide. An efficient H-D exchange reaction was observed, which gave various deuterium-labeled aromatic compds.

IT 1314-15-4, Platinum(IV) oxide
RL: CAT (Catalyst use); USES (Uses)
(platinum-catalyzed hydrothermal hydrogen-deuterium exchange of aromatic compds.)
RN 1314-15-4 CAPLUS
CN Platinum oxide (PtO2) (CA INDEX NAME)



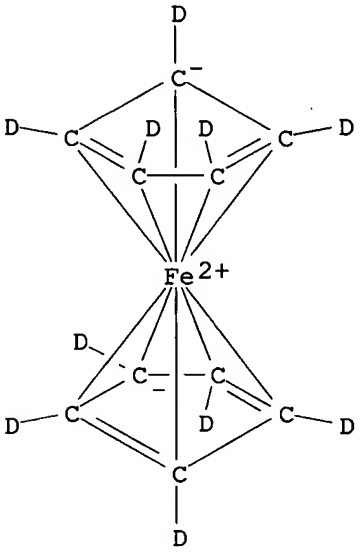
IT 63683-54-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(platinum-catalyzed hydrothermal hydrogen-deuterium exchange of aromatic compds.)
RN 63683-54-5 CAPLUS
CN Phosphine, tri(phenyl-2,6-d2)- (9CI) (CA INDEX NAME)



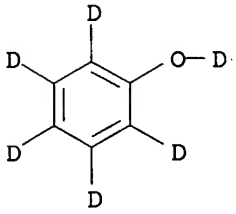

IT 12082-87-0P, Ferrocene-d10 13127-88-3P, Phenol-d6
17157-12-9P, Isoquinoline-d7 20617-93-0P, Quinoxaline-d6
32190-42-4P 34071-94-8P, Quinoline-d7
54964-93-1P 73509-20-3P, 1H-Indole-1,2,3,4,5,6,7-d7
93952-05-7P 97960-58-2P 132125-39-4P

634897-78-2P 880462-19-1P 880462-20-4P
880462-21-5P 880462-22-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(platinum-catalyzed hydrothermal hydrogen-deuterium exchange of aromatic compds.)

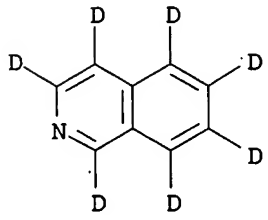
RN 12082-87-0 CAPLUS
CN Ferrocene-d10 (8CI, 9CI) (CA INDEX NAME)



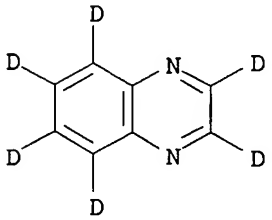
RN 13127-88-3 CAPLUS
CN Phen-2,3,4,5,6-d5-ol-d (CA INDEX NAME)



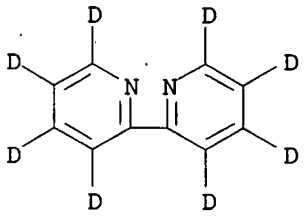
RN 17157-12-9 CAPLUS
CN Isoquinoline-1,3,4,5,6,7,8-d7 (CA INDEX NAME)



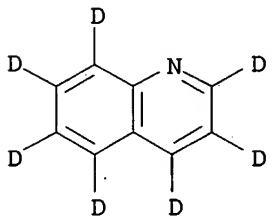
RN 20617-93-0 CAPLUS
CN Quinoxaline-2,3,5,6,7,8-d6 (CA INDEX NAME)



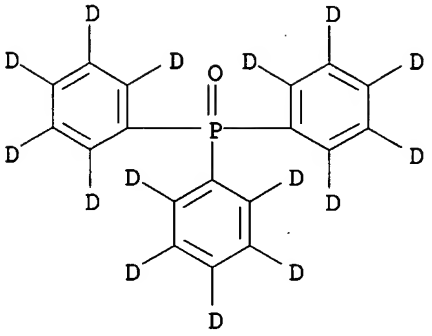
RN 32190-42-4 CAPLUS
CN 2,2'-Bipyridine-3,3',4,4',5,5',6,6'-d8 (CA INDEX NAME)



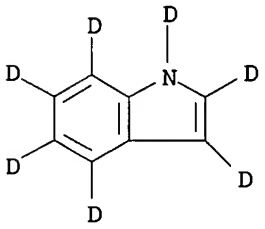
RN 34071-94-8 CAPLUS
CN Quinoline-2,3,4,5,6,7,8-d7 (CA INDEX NAME)



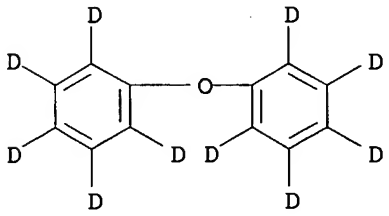
RN 54964-93-1 CAPLUS
CN Phosphine oxide, tri(phenyl-d5)- (9CI) (CA INDEX NAME)



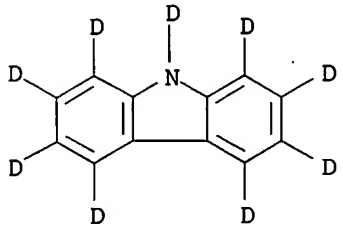
RN 73509-20-3 CAPLUS
CN 1H-Indole-1,2,3,4,5,6,7-d7 (CA INDEX NAME)



RN 93952-05-7 CAPLUS
CN Benzene-d5, 6,6'-oxybis- (9CI) (CA INDEX NAME)

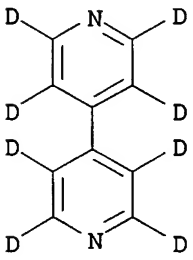


RN 97960-58-2 CAPLUS
CN 9H-Carbazole-1,2,3,4,5,6,7,8,9-d9 (CA INDEX NAME)

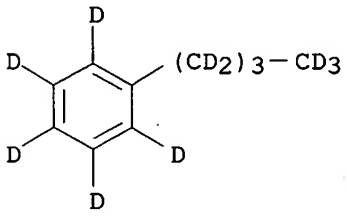


RN 132125-39-4 CAPLUS

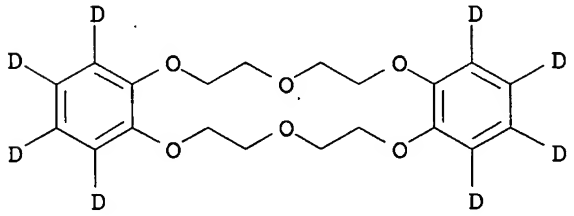
CN 4,4'-Bipyridine-2,2',3,3',5,5',6,6'-d8 (CA INDEX NAME)



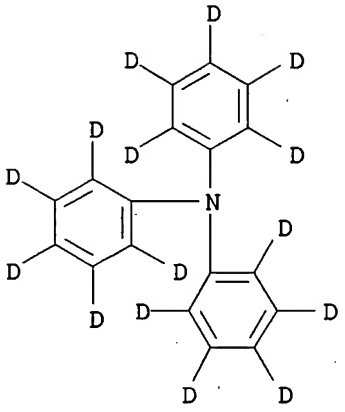
RN 634897-78-2 CAPLUS
CN Benzene-1,2,3,4,5-d5, 6-(butyl-1,1,2,2,3,3,4,4,4-d9)- (CA INDEX NAME)



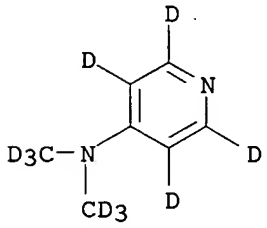
RN 880462-19-1 CAPLUS
CN Dibenzo[b,k][1,4,7,10,13,16]hexaoxacyclooctadecin-1,2,3,4,12,13,14,15-d8, 6,7,9,10,17,18,20,21-octahydro- (8CI, 9CI) (CA INDEX NAME)



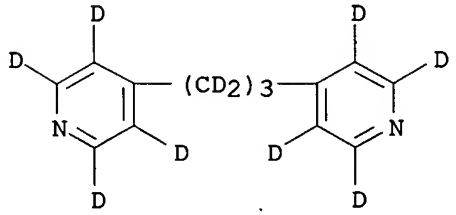
RN 880462-20-4 CAPLUS
CN Benzen-d5-amine, N,N-di(phenyl-d5)- (9CI) (CA INDEX NAME)



RN 880462-21-5 CAPLUS
CN 4-Pyridin-2,3,5,6-d4-amine, N,N-di(methyl-d3)- (9CI) (CA INDEX NAME)



RN 880462-22-6 CAPLUS
CN Pyridine-2,3,5,6-d4, 4,4'-(1,3-propanediyl-1,1,2,2,3,3-d6)bis- (CA INDEX NAME)



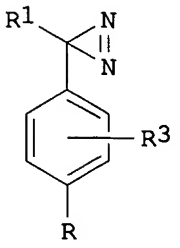
REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 13 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:982579 CAPLUS
DOCUMENT NUMBER: 143:286411
TITLE: Preparation of deuterated diazirine compounds
INVENTOR(S): Hashimoto, Makoto; Hatanaka, Yasumaru
PATENT ASSIGNEE(S): Japan Science and Technology Agency, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 11 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent

LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| JP 2005239577 | A | 20050908 | JP 2004-48176 | 20040224 |

PRIORITY APPLN. INFO.: JP 2004-48176 20040224
OTHER SOURCE(S): MARPAT 143:286411
GI

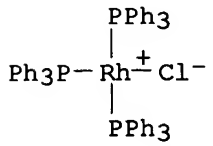


I

AB The compds. I [R = CHX1CHR2X2; R1 = (fluoro)alkyl; R2 = H, alkyl, carboxyl, CO2R4 (R4 = alkyl, aralkyl); R3 = H, alkoxy, O(CmH2mO)n(CH2)oR5 (m = 2, 3; n = 1-6; o = 1-4; R5 = H, carboxyl, amino, OH); X1, X2 = H, D; X1 and/or X2 = deuterium] (II), useful as photoaffinity labels for anal. of biopolymers, are prepared by deuteration of I (R = CH:CR6R7; one of R6 and R7 = same as R2 and the other = H) (III) using Wilkinson's catalyst. Thus, III (R1 = CF3, R6 = CO2Et, R3 = R7 = H), prepared from 4-bromobenzene with 6 steps, was dissolved in THF/Me3COH and stirred under a deuterium atmospheric at room temperature for 5 h to give II (R1 = CF3, R2 = CO2Et, X1 = X2 = D; R3 = H).

IT 14694-95-2, Wilkinson's catalyst
RL: CAT (Catalyst use); USES (Uses)
(preparation of deuterated diazirine compds. as photoaffinity labels by deuteration of (vinylphenyl)diazirines using Wilkinson's catalyst)

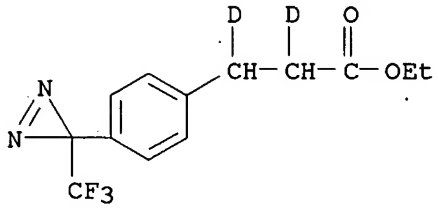
RN 14694-95-2 CAPLUS
CN Rhodium, chlorotris(triphenylphosphine)-, (SP-4-2)- (CA INDEX NAME)



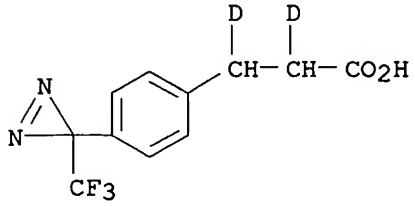
IT 864235-86-9P 864235-88-1P 864235-90-5P
864235-92-7P
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of deuterated diazirine compds. as photoaffinity labels by deuteration of (vinylphenyl)diazirines using Wilkinson's catalyst)

RN 864235-86-9 CAPLUS
CN Benzenepropanoic-α,β-d2 acid, 4-[3-(trifluoromethyl)-3H-

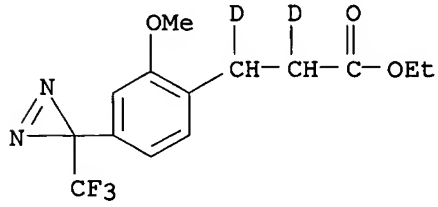
diazirin-3-yl]-, ethyl ester (CA INDEX NAME)



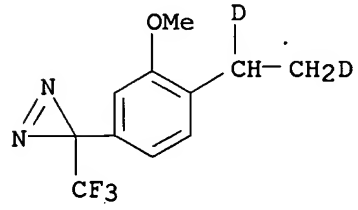
RN 864235-88-1 CAPLUS
CN Benzenepropanoic-α,β-d2 acid, 4-[3-(trifluoromethyl)-3H-diazirin-3-yl]- (9CI) (CA INDEX NAME)



RN 864235-90-5 CAPLUS
CN Benzenepropanoic-α,β-d2 acid, 2-methoxy-4-[3-(trifluoromethyl)-3H-diazirin-3-yl]-, ethyl ester (CA INDEX NAME)



RN 864235-92-7 CAPLUS
CN 3H-Diazirine, 3-[4-(ethyl-1,2-d2)-3-methoxyphenyl]-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



L24 ANSWER 14 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:980492 CAPLUS
DOCUMENT NUMBER: 143:439970

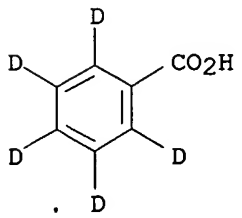
TITLE: Aromatic ring favorable and efficient H-D exchange reaction catalyzed by Pt/C
AUTHOR(S): Sajiki, Hironao; Ito, Nobuhiro; Esaki, Hiroyoshi; Maesawa, Tsuneaki; Maegawa, Tomohiro; Hirota, Kosaku
CORPORATE SOURCE: Laboratory of Medicinal Chemistry, Gifu Pharmaceutical University, Gifu, 502-8585, Japan
SOURCE: Tetrahedron Letters (2005), 46(41), 6995-6998
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 143:439970

AB An effective and applicable Pt/C-catalyzed deuteration method of aromatic rings using D2O as a deuterium source under hydrogen atmospheric was developed. Five percent Pt/C would lead to quite effective H-D exchange results on the aromatic ring systems. The reaction is general for a variety of aromatic compds. including biol. active compds.

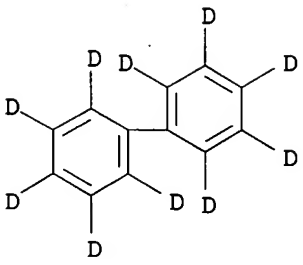
IT 7440-06-4, Platinum, uses
RL: CAT (Catalyst use); USES (Uses)
(preparation of deuterated arene derivs. via efficient platinum/carbon catalyzed hydrogen-deuterium exchange reaction using deuterium oxide as reactant)
RN 7440-06-4 CAPLUS
CN Platinum (CA INDEX NAME)

Pt

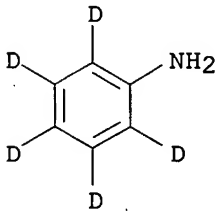
IT 1079-02-3P, Benzoic-d5 acid 1486-01-7P
4165-61-1P, Benzen-d5-amine 4165-62-2P, Phen-d5-ol
85921-99-9P, preparation 87976-26-9P 97964-46-0P
, preparation 103963-58-2P, 1,2-Benzene-3,4,5,6-d4-diol
121887-11-4P 291765-93-0P, 1,2-Benzene-3,4,5,6-d4-diamine 651316-70-0P 868699-74-5P 868699-77-8P
868699-78-9P 868699-84-7P, preparation
868699-87-0P, preparation 868699-95-0P, preparation
868699-96-1P 868759-42-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of deuterated arene derivs. via efficient platinum/carbon catalyzed hydrogen-deuterium exchange reaction using deuterium oxide as reactant)
RN 1079-02-3 CAPLUS
CN Benzoic-2,3,4,5,6-d5 acid (CA INDEX NAME)



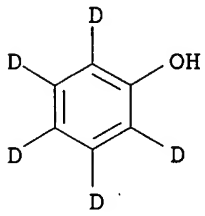

RN 1486-01-7 CAPLUS
CN 1,1'-Biphenyl-2,2',3,3',4,4',5,5',6,6'-d10 (CA INDEX NAME)



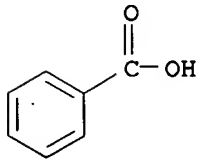
RN 4165-61-1 CAPLUS
CN Benzen-2,3,4,5,6-d5-amine (CA INDEX NAME)



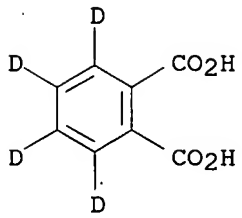
RN 4165-62-2 CAPLUS
CN Phen-2,3,4,5,6-d5-ol (CA INDEX NAME)



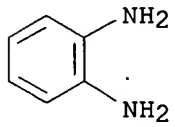
RN 85921-99-9 CAPLUS
CN Benzoic acid, labeled with deuterium (9CI) (CA INDEX NAME)



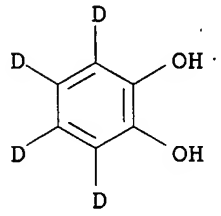
RN 87976-26-9 CAPLUS
CN 1,2-Benzene-3,4,5,6-d4-dicarboxylic acid (9CI) (CA INDEX NAME)



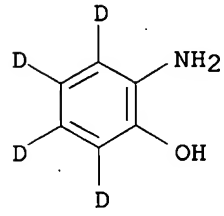
RN 97964-46-0 CAPLUS
CN 1,2-Benzenediamine, labeled with deuterium (9CI) (CA INDEX NAME)



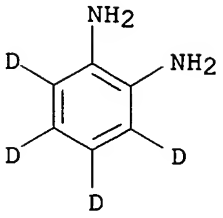
RN 103963-58-2 CAPLUS
CN 1,2-Benzene-3,4,5,6-d4-diol (9CI) (CA INDEX NAME)



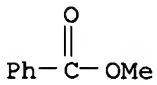
RN 121887-11-4 CAPLUS
CN Phen-2,3,4,5-d4-ol, 6-amino- (9CI) (CA INDEX NAME)



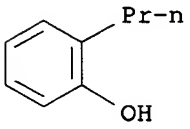
RN 291765-93-0 CAPLUS
CN 1,2-Benzene-3,4,5,6-d4-diamine (9CI) (CA INDEX NAME)



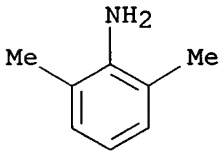
RN 651316-70-0 CAPLUS
CN Benzoic acid, methyl ester, labeled with deuterium (9CI) (CA INDEX NAME)



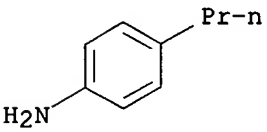
RN 868699-74-5 CAPLUS
CN Phenol, 2-propyl-, labeled with deuterium (9CI) (CA INDEX NAME)



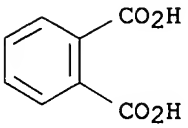
RN 868699-77-8 CAPLUS
CN Benzenamine, 2,6-dimethyl-, labeled with deuterium (9CI) (CA INDEX NAME)



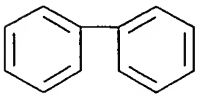
RN 868699-78-9 CAPLUS
CN Benzenamine, 4-propyl-, labeled with deuterium (9CI) (CA INDEX NAME)



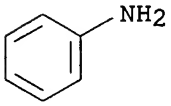
RN 868699-84-7 CAPLUS
CN 1,2-Benzenedicarboxylic acid, labeled with deuterium (9CI) (CA INDEX NAME)



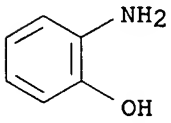
RN 868699-87-0 CAPLUS
CN 1,1'-Biphenyl, labeled with deuterium (9CI) (CA INDEX NAME)



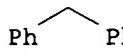
RN 868699-95-0 CAPLUS
CN Benzenamine, labeled with deuterium (9CI) (CA INDEX NAME)



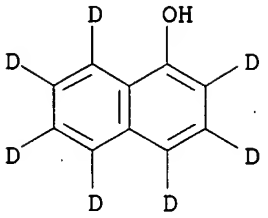
RN 868699-96-1 CAPLUS
CN Phenol, 2-amino-, labeled with deuterium (9CI) (CA INDEX NAME)



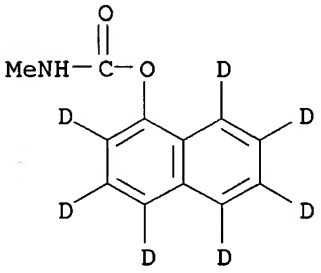
RN 868759-42-6 CAPLUS
CN Benzene, 1,1'-methylenebis-, labeled with deuterium (9CI) (CA INDEX NAME)



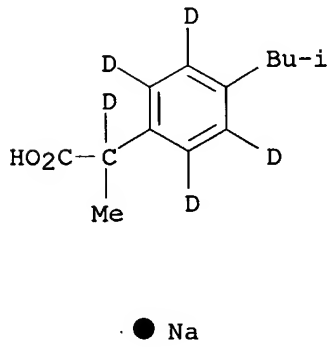
IT 124251-84-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of deuterated naphthalenyl carbamate via efficient platinum/carbon catalyzed hydrogen-deuterium exchange reaction using deuterium oxide as reactant)
RN 124251-84-9 CAPLUS
CN 1-Naphthalen-2,3,4,5,6,7,8-d7-ol (CA INDEX NAME)



IT 362049-56-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of deuterated naphthalenyl carbamate via efficient platinum/carbon catalyzed hydrogen-deuterium exchange reaction using deuterium oxide as reactant)
RN 362049-56-7 CAPLUS
CN 1-Naphthalen-2,3,4,5,6,7,8-d7-ol, methylcarbamate (9CI) (CA INDEX NAME)



IT 868699-91-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of ibuprofen-d17 via efficient platinum/carbon catalyzed hydrogen-deuterium exchange reaction using deuterium oxide as reactant)
RN 868699-91-6 CAPLUS
CN Benzene-2,3,5,6-d4-acetic-α-d acid, α-methyl-4-(2-methylpropyl)-, labeled with deuterium, sodium salt (9CI) (CA INDEX NAME)



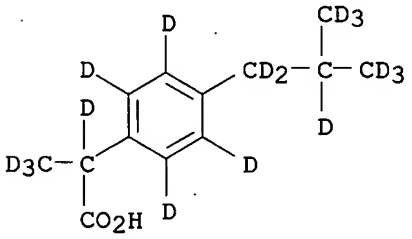


IT 868699-93-8P 868699-94-9P
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of ibuprofen-d17 via efficient platinum/carbon catalyzed hydrogen-deuterium exchange reaction using deuterium oxide as reactant)

RN 868699-93-8 CAPLUS

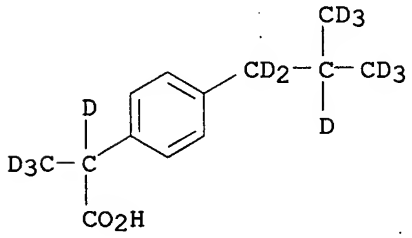
CN Benzene-2,3,5,6-d4-acetic-α-d acid, α-(methyl-d3)-4-[2-(methyl-d3)propyl-1,1,2,3,3,3-d6]-, sodium salt (9CI) (CA INDEX NAME)



● Na

RN 868699-94-9 CAPLUS

CN Benzeneacetic-α-d acid, α-(methyl-d3)-4-[2-(methyl-d3)propyl-1,1,2,3,3,3-d6]-, sodium salt (1:1) (CA INDEX NAME)



● Na

REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 15 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:945100 CAPLUS

DOCUMENT NUMBER: 143:422450

TITLE: Stoichiometric and Catalytic sp3 C-H/D2 Exchange Reactions of ortho-Substituted Benzenethiol and Phenols by a Ruthenium(II) Complex. Effect of a Chalcogen Anchor on the Bond Cleavage Reaction

AUTHOR(S): Hirano, Masafumi; Sakaguchi, Yuko; Yajima, Toshiaki; Kurata, Naoki; Komine, Nobuyuki; Komiya, Sanshiro

CORPORATE SOURCE: Department of Applied Chemistry, Graduate School of Engineering, Tokyo University of Agriculture and Technology, 2-24-16 Koganei, Tokyo, 184-8588, Japan

SOURCE: Organometallics (2005), 24(20), 4799-4809
CODEN: ORGND7; ISSN: 0276-7333

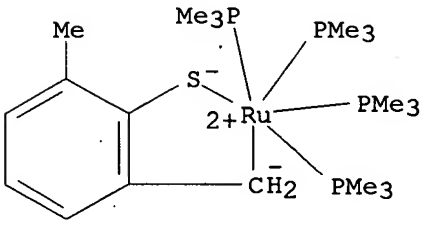
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 143:422450

AB 2,6-Dimethylbenzenethiol and 2,6-dimethylphenol undergo cyclometalation and hydrogen-deuterium exchange with ruthenium(0) cycloalkene and trimethylphosphine complexes; crystal structure and kinetics of formation of the cyclometalated species were determined Reaction of Ru(η4-1,5-COD)(η6-1,3,5-COT) (1) with 2,6-dimethylbenzenethiol and PMe3 afforded Ru(II) thiaruthenacycle complex, cis-Ru[SC6H3(2-CH2)(6-Me)-κ2S,C](PMe3)4 (3), via intermediate Ru(η5-cyclooctadienyl)(SC6H3Me2-2,6)(PMe3)2 (2). Exposure of 3 to H2 (0.1 MPa) in benzene leads to the quant. formation of cis-RuH(SC6H3Me2-2,6)(PMe3)4 (4), which readily turns to 3 at room temperature on evacuation, indicating the reversibility of the reaction. Both forward and backward reactions of this equilibrium are retarded by addition of PMe3, suggesting prerequisite prior dissociation of PMe3 for both reactions. Complex 3 catalyzes selective and facile deuteration of the ortho-Me and the mercapto groups in 2,6-dimethylbenzenethiol by D2 gas.

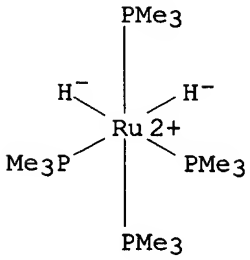
IT 868257-99-2P
RL: CAT (Catalyst use); CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent); USES (Uses)
(crystal structure; reversible hydrogenolysis of ruthenium cyclometalated 2,6-dimethylbenzenethiolates in preparation of hydride regioselective Me group deuteration catalysts)

RN 868257-99-2 CAPLUS
CN Ruthenium, [2-(methyl-κC)-6-methylbenzenethiolato(2-)-κS]tetrakis(trimethylphosphine)-, (OC-6-23)- (9CI) (CA INDEX NAME)

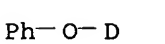



IT 76171-49-8P
RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(reversible hydrogenolysis of ruthenium cyclometalated 2,6-dimethylbenzenethiolates in preparation of hydride regioselective Me group deuteration catalysts)

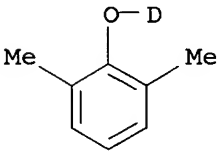
RN 76171-49-8 CAPLUS
CN Ruthenium, dihydrotetrakis(trimethylphosphine)-, (OC-6-22)- (CA INDEX NAME)



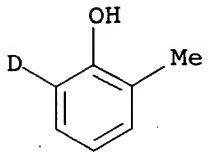

IT 1003-66-3P, Phenol-d 22100-62-5P 219822-08-9P
854927-24-5P 868258-01-9P 868258-02-0P
868258-03-1P 868258-04-2P 868258-05-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(reversible hydrogenolysis of ruthenium cyclometalated
2,6-dimethylbenzenethiolates in preparation of hydride regioselective Me
group deuteration catalysts)
RN 1003-66-3 CAPLUS
CN Phenol-d (CA INDEX NAME)



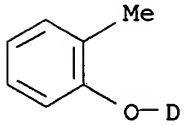

RN 22100-62-5 CAPLUS
CN Phenol-d, 2,6-dimethyl- (9CI) (CA INDEX NAME)



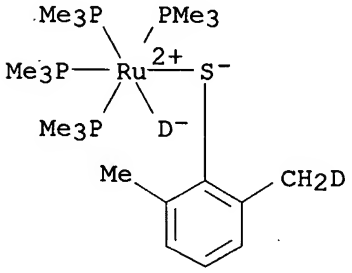

RN 219822-08-9 CAPLUS
CN Phen-2-d-ol, 6-methyl- (9CI) (CA INDEX NAME)



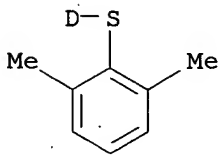

RN 854927-24-5 CAPLUS
CN Phenol-d, 2-methyl- (9CI) (CA INDEX NAME)



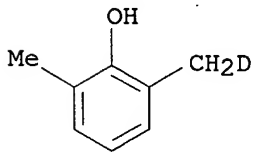
RN 868258-01-9 CAPLUS
CN Ruthenium, hydro-d-[2-methyl-6-(methyl-d)benzenethiolato]tetrakis(trimethylphosphine)-, (OC-6-23)- (9CI) (CA INDEX NAME)



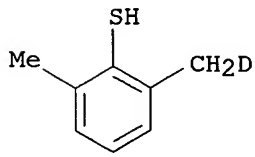

RN 868258-02-0 CAPLUS
CN Benzenethiol-d, 2,6-dimethyl- (9CI) (CA INDEX NAME)



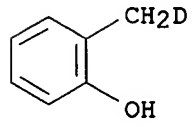

RN 868258-03-1 CAPLUS
CN Phenol, 2-methyl-6-(methyl-d)- (9CI) (CA INDEX NAME)




RN 868258-04-2 CAPLUS
CN Benzenethiol, 2-methyl-6-(methyl-d)- (9CI) (CA INDEX NAME)




RN 868258-05-3 CAPLUS
CN Phenol, 2-(methyl-d)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 70 THERE ARE 70 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 16 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:696848 CAPLUS
DOCUMENT NUMBER: 143:172769
TITLE: Method of deuteration of aromatic ring and/or heterocycle compounds using mixed metal catalyst
INVENTOR(S): Ito, Nobuhiro; Maesawa, Tsuneaki; Muto, Kazushige; Hirota, Kosaku; Sajiki, Hironao
PATENT ASSIGNEE(S): Wako Pure Chemical Industries, Ltd., Japan
SOURCE: PCT Int. Appl., 55 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2005070853 | A1 | 20050804 | WO 2004-JP19049 | 20041221 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW | | | | |
| RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| CA 2553376 | A1 | 20050804 | CA 2004-2553376 | 20041221 |
| EP 1707548 | A1 | 20061004 | EP 2004-807406 | 20041221 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, IS | | | | |
| CN 1906143 | A | 20070131 | CN 2004-80040874 | 20041221 |
| PRIORITY APPLN. INFO.: | | | JP 2004-16075 A | 20040123 |
| | | | WO 2004-JP19049 W | 20041221 |

AB A method of deuteration in which a compound with aromatic ring and/or heterocycle having an enhanced deuteration ratio can be obtained. There is provided a method of deuterating a compound with aromatic ring and/or heterocycle, characterized in that a compound with aromatic ring and/or heterocycle is reacted with a deuterium source in the presence of an activated mixed catalyst composed of at least two members selected from among a palladium catalyst, a platinum catalyst, a rhodium catalyst, an iridium catalyst, a ruthenium catalyst, a nickel catalyst and a cobalt catalyst. Thus, 500 mg nicotinic acid, 50 mg Pd/C (5 mg Pd), and 100 mg Pt/C (5 mg Pt) were suspended in 17 mL D2O, sealed, purged with H, and heated at 180° for .apprx.24 h to give deuterated nicotinic acid with 99% deuteration at 2, 5, and 6 positions and 48% deuteration at 4 position vs. 98% deuteration at 2 and 5 positions, 99% deuteration at 6 position, and 10% deuteration at 4 position when Pd/C was used alone.

IT 7440-02-0, Nickel, uses 7440-06-4, Platinum, uses 7440-06-4D, Platinum, supported on carbon 7440-16-6, Rhodium, uses 7440-18-8, Ruthenium, uses 7440-48-4, Cobalt, uses

RL: CAT (Catalyst use); USES (Uses)
(method of deuteration of aromatic ring and/or heterocycle compds. using mixed metal catalyst such as palladium and platinum on carbon)
RN 7440-02-0 CAPLUS
CN Nickel (CA INDEX NAME)

Ni

RN 7440-06-4 CAPLUS
CN Platinum (CA INDEX NAME)

Pt

RN 7440-06-4 CAPLUS
CN Platinum (CA INDEX NAME)

Pt

RN 7440-16-6 CAPLUS
CN Rhodium (CA INDEX NAME)

Rh

RN 7440-18-8 CAPLUS
CN Ruthenium (CA INDEX NAME)

Ru

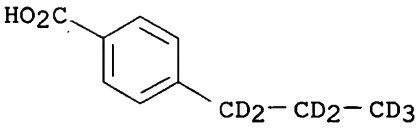
RN 7440-48-4 CAPLUS
CN Cobalt (CA INDEX NAME)

Co

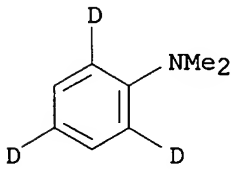
IT 7128-85-0P 7217-47-2DP, deuterated derivative
22527-01-1DP, deuterated derivative 22527-01-1P
66148-15-0P 87385-38-4DP, deuterated derivative
134860-14-3DP, Benzenebutanoic-α,α,β,β,.gamm
a.,γ-d6 acid, deuterated derivative 358730-86-6P,
Benzene-d5-butanoic-d6 acid 767627-97-4P, Benzene-d5-pentanoic-
d8 acid 861405-57-4DP, Benzenepentanoic-d8 acid, deuterated
derivative 861405-58-5DP, Benzene-3,4,5-d3-pentanoic acid,
deuterated derivative 861405-59-6DP, deuterated derivative
861405-60-9DP, Benzene-3,4,5-d3-butanoic acid, deuterated derivative
861405-61-0DP, deuterated derivative 861405-62-1P
861405-63-2P 861405-64-3DP, deuterated derivative
861405-65-4P 861405-66-5DP, deuterated derivative

861405-67-6DP, deuterated derivative 861405-68-7P
861405-69-8P 861405-70-1DP, deuterated derivative
861405-71-2P 861405-72-3P 861405-73-4DP,
deuterated derivative 861405-74-5DP, deuterated derivative
861405-75-6P 861405-76-7DP, 3-Pyridine-6-d-carboxylic
acid, deuterated derivative
RL: SPN (Synthetic preparation); PREP (Preparation)
(method of deuteration of aromatic ring and/or heterocycle compds. using mixed metal catalyst such as palladium and platinum on carbon)

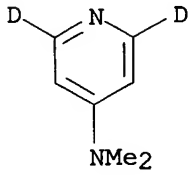
RN 7128-85-0 CAPLUS
CN Benzoic acid, 4-(propyl-d7)- (9CI) (CA INDEX NAME)



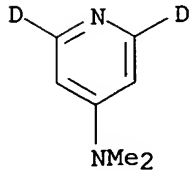
RN 7217-47-2 CAPLUS
CN Benzen-2,4,6-d3-amine, N,N-dimethyl- (9CI) (CA INDEX NAME)



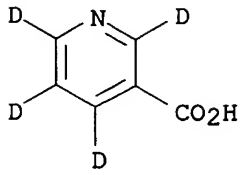
RN 22527-01-1 CAPLUS
CN 4-Pyridin-2,6-d2-amine, N,N-dimethyl- (9CI) (CA INDEX NAME)



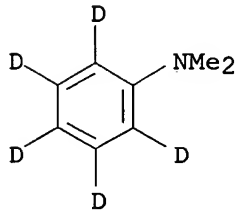
RN 22527-01-1 CAPLUS
CN 4-Pyridin-2,6-d2-amine, N,N-dimethyl- (9CI) (CA INDEX NAME)



RN 66148-15-0 CAPLUS
CN 3-Pyridine-2,4,5,6-d4-carboxylic acid (9CI) (CA INDEX NAME)



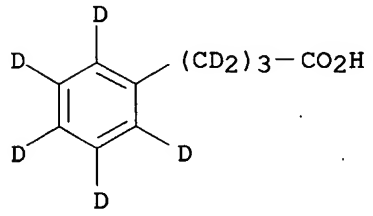
RN 87385-38-4 CAPLUS
CN Benzen-d5-amine, N,N-dimethyl- (9CI) (CA INDEX NAME)



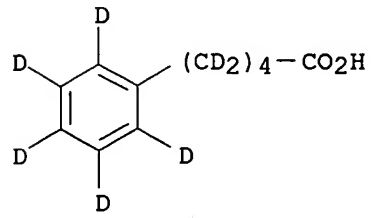
RN 134860-14-3 CAPLUS
CN Benzenebutanoic-α,α,β,β,γ,γ-d6 acid (9CI) (CA INDEX NAME)

Ph—$(CD_2)_3$—$CO_2H$

RN 358730-86-6 CAPLUS
CN Benzene-d5-butanoic-d6 acid (9CI) (CA INDEX NAME)



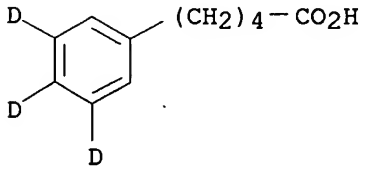
RN 767627-97-4 CAPLUS
CN Benzene-d5-pentanoic-d8 acid (CA INDEX NAME)



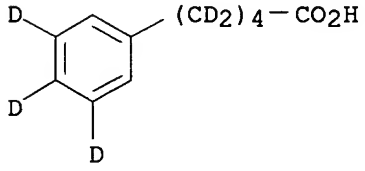
RN 861405-57-4 CAPLUS
CN Benzenepentanoic-d8 acid (9CI) (CA INDEX NAME)

Ph—$(CD_2)_4$—$CO_2H$

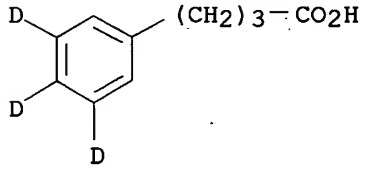
RN 861405-58-5 CAPLUS
CN Benzene-3,4,5-d3-pentanoic acid (9CI) (CA INDEX NAME)



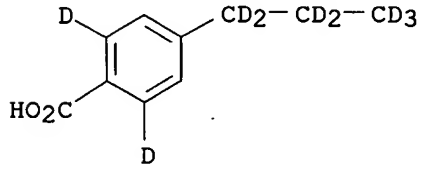
RN 861405-59-6 CAPLUS
CN Benzene-3,4,5-d3-pentanoic-α,α,β,β,γ,γ,.
delta.,δ-d8 acid (9CI) (CA INDEX NAME)



RN 861405-60-9 CAPLUS
CN Benzene-3,4,5-d3-butanoic acid (9CI) (CA INDEX NAME)

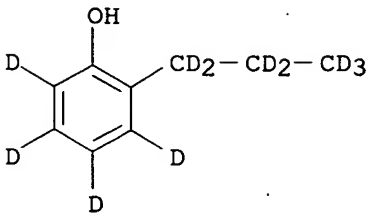


RN 861405-61-0 CAPLUS
CN Benzoic-2,6-d2 acid, 4-(propyl-d7)- (9CI) (CA INDEX NAME)

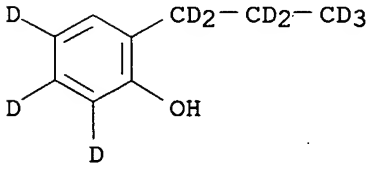


RN 861405-62-1 CAPLUS

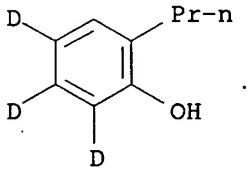
CN Phen-2,3,4,5-d4-ol, 6-(propyl-d7)- (CA INDEX NAME)



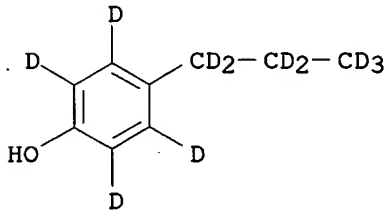
RN 861405-63-2 CAPLUS
CN Phen-2,3,4-d3-ol, 6-(propyl-d7)- (9CI) (CA INDEX NAME)



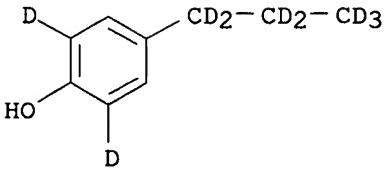
RN 861405-64-3 CAPLUS
CN Phen-2,3,4-d3-ol, 6-propyl- (9CI) (CA INDEX NAME)



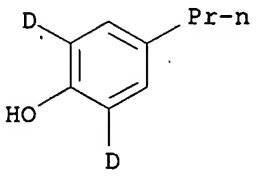
RN 861405-65-4 CAPLUS
CN Phen-2,3,5,6-d4-ol, 4-(propyl-d7)- (9CI) (CA INDEX NAME)



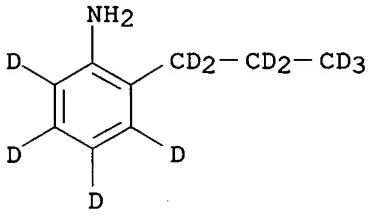
RN 861405-66-5 CAPLUS
CN Phen-2,6-d2-ol, 4-(propyl-d7)- (9CI) (CA INDEX NAME)



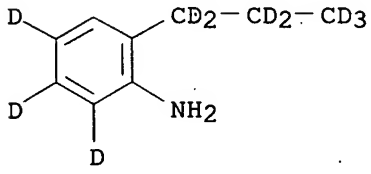
RN 861405-67-6 CAPLUS
CN Phen-2,6-d2-ol, 4-propyl- (9CI) (CA INDEX NAME)



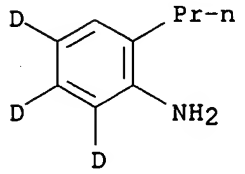
RN 861405-68-7 CAPLUS
CN Benzen-2,3,4,5-d4-amine, 6-(propyl-d7)- (9CI) (CA INDEX NAME)



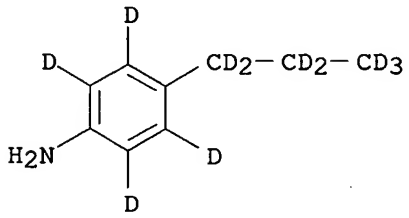
RN 861405-69-8 CAPLUS
CN Benzen-2,3,4-d3-amine, 6-(propyl-d7)- (9CI) (CA INDEX NAME)



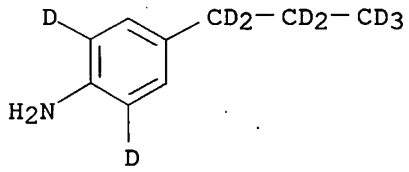
RN 861405-70-1 CAPLUS
CN Benzen-2,3,4-d3-amine, 6-propyl- (9CI) (CA INDEX NAME)



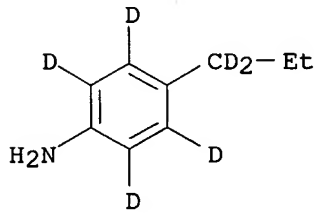
RN 861405-71-2 CAPLUS
CN Benzen-2,3,5,6-d4-amine, 4-(propyl-d7)- (9CI) (CA INDEX NAME)



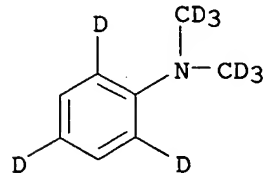
RN 861405-72-3 CAPLUS
CN Benzen-2,6-d2-amine, 4-(propyl-d7)- (9CI) (CA INDEX NAME)



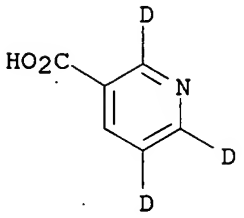
RN 861405-73-4 CAPLUS
CN Benzen-2,3,5,6-d4-amine, 4-(propyl-1,1-d2)- (9CI) (CA INDEX NAME)



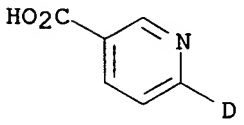
RN 861405-74-5 CAPLUS
CN Benzen-2,4,6-d3-amine, N,N-di(methyl-d3)- (9CI) (CA INDEX NAME)



RN 861405-75-6 CAPLUS
CN 3-Pyridine-2,5,6-d3-carboxylic acid (CA INDEX NAME)

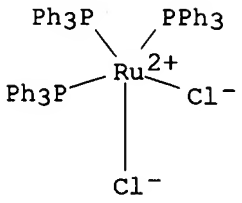


RN 861405-76-7 CAPLUS
CN 3-Pyridine-6-d-carboxylic acid (9CI) (CA INDEX NAME)

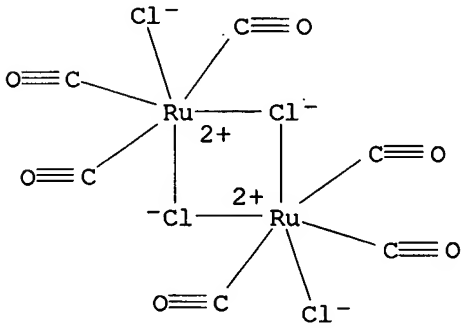


REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 17 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:460973 CAPLUS
DOCUMENT NUMBER: 143:152841
TITLE: One-step exchange-labeling of piperidines, piperazines and dialkylamines with deuterium oxide: catalysis by various ruthenium complexes
AUTHOR(S): Alexakis, Efstathios; Hickey, Michael J.; Jones, John R.; Kingston, Lee P.; Lockley, William J. S.; Mather, Andrew N.; Smith, Traci; Wilkinson, David J.
CORPORATE SOURCE: School of Biomedical and Molecular Sciences, Department of Chemistry, University of Surrey, Surrey, Guildford, GU2 7XH, UK
SOURCE: Tetrahedron Letters (2005), 46(25), 4291-4293
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 143:152841
AB A range of variously substituted piperidines, piperazines, and dialkylamines can be conveniently deuterated in a single step by isotopic exchange with deuterium oxide in the presence of an appropriate ruthenium complex catalyst. The isotopic exchange can be carried out efficiently in DMSO; hence it is directly applicable to the deuteration of polar compds. such as pharmaceuticals. Isotopic incorporations are high, while recoveries are variable and generally moderate. Deuteration takes place at positions both α and β to the NH group.
IT 15529-49-4, Tris(triphenylphosphine)ruthenium dichloride
22594-69-0 37366-09-9
RL: CAT (Catalyst use); USES (Uses)
(one-step exchange-labeling of piperidines, piperazines, and dialkylamines with deuterium oxide catalyzed by ruthenium complexes)
RN 15529-49-4 CAPLUS
CN Ruthenium, dichlorotris(triphenylphosphine)- (CA INDEX NAME)

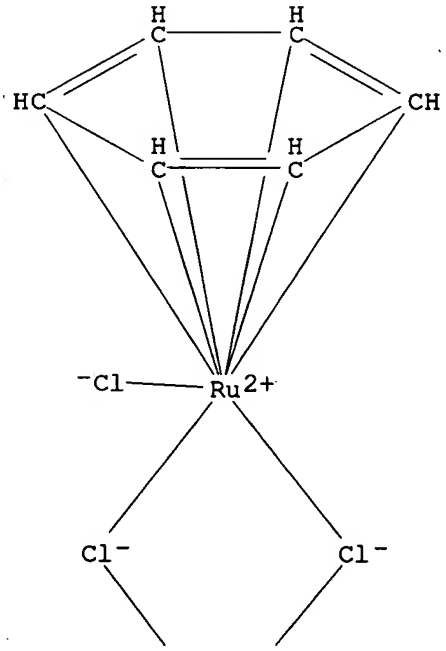


RN 22594-69-0 CAPLUS
CN Ruthenium, hexacarbonyldi-μ-chlorodichlorodi- (CA INDEX NAME)

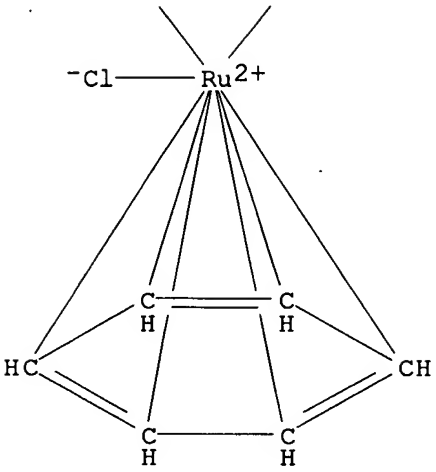


RN 37366-09-9 CAPLUS
CN Ruthenium, bis(η6-benzene)di-μ-chlorodichlorodi- (CA INDEX NAME)

PAGE 1-A



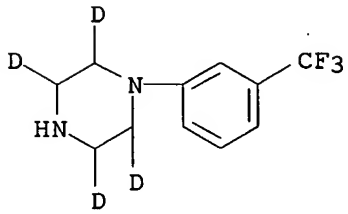
PAGE 2-A




IT 859843-14-4P 860027-49-2P 860027-50-5P
860027-51-6P 860027-52-7P 860027-53-8P
860027-54-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(one-step exchange-labeling of piperidines, piperazines, and dialkylamines with deuterium oxide catalyzed by ruthenium complexes)
RN 859843-14-4 CAPLUS
CN Piperazine-2,3,5,6-d4, 1-[3-(trifluoromethyl)phenyl]-, ethanedioate (1:1) (9CI) (CA INDEX NAME)

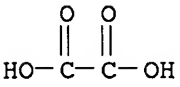
CM 1

CRN 859843-13-3
CMF C11 H9 D4 F3 N2

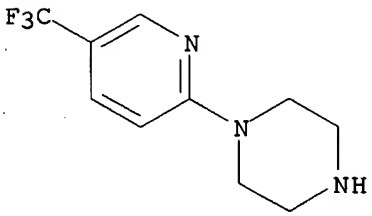



CM 2

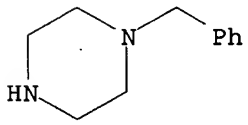
CRN 144-62-7
CMF C2 H2 O4



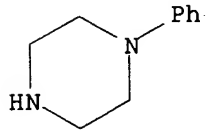
RN 860027-49-2 CAPLUS
CN Piperazine, 1-[5-(trifluoromethyl)-2-pyridinyl]-, labeled with deuterium (9CI) (CA INDEX NAME)



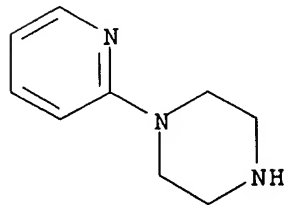
RN 860027-50-5 CAPLUS
CN Piperazine, 1-(phenylmethyl)-, labeled with deuterium (9CI) (CA INDEX NAME)



RN 860027-51-6 CAPLUS
CN Piperazine, 1-phenyl-, labeled with deuterium (9CI) (CA INDEX NAME)

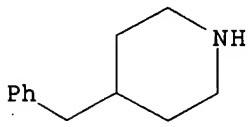


RN 860027-52-7 CAPLUS
CN Piperazine, 1-(2-pyridinyl)-, labeled with deuterium (9CI) (CA INDEX NAME)

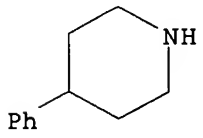


RN 860027-53-8 CAPLUS

CN Piperidine, 4-(phenylmethyl)-, labeled with deuterium (9CI) (CA INDEX NAME)




RN 860027-54-9 CAPLUS
CN Piperidine, 4-phenyl-, labeled with deuterium (9CI) (CA INDEX NAME)



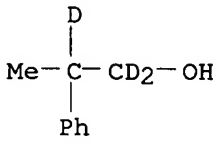

REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 18 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:144103 CAPLUS
DOCUMENT NUMBER: 142:373493
TITLE: Ruthenium catalyzed deuterium labeling of α-carbon in primary alcohol and primary/secondary amine in D2O
AUTHOR(S): Takahashi, Masaaki; Oshima, Koichiro; Matsubara, Seijiro
CORPORATE SOURCE: Department of Material Chemistry, Graduate School of Engineering, Kyoto University, Kyoto, 615-8510, Japan
SOURCE: Chemistry Letters (2005), 34(2), 192-193
CODEN: CMLTAG; ISSN: 0366-7022
PUBLISHER: Chemical Society of Japan
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:373493

AB Primary alcs. and primary/secondary amines are labeled with deuterium atom at α-position regioselectively by means of deuterium oxide and ruthenium catalyst. For example, the microwave-mediated ruthenium-catalyzed deuteration of (1S,2S,5S)-6,6-dimethylbicyclo[3.1.1]heptane-2-methanol (myrtanol) gave (1S,2S,5S)-6,6-dimethylbicyclo[3.1.1]heptane-2-methan-α,α-d2-ol. Deuteration at the β-position could be suppressed, if the reaction was carried out below 100° with the use of microwaves. In the case of primary amines H-D-exchange was observed at the α-position selectively. a work-up with NaOD gave high contents of deuterium on nitrogen as well. H-D-exchange on a tertiary amine gave only a small amount of exchanged product.

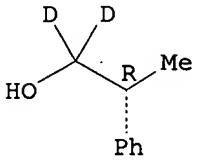
IT 849700-25-0P
RL: BYP (Byproduct); PREP (Preparation)
(preparation of (R)-β-(methyl)benzenemethan-α,α-d2-ol and β-deuterated isomer by deuterium labeling using (phenyl)propanol and deuterium oxide as starting materials and dichlorobis(triphenylphosphine)ruthenium as catalyst)

RN 849700-25-0 CAPLUS
CN Benzeneethan-α,α,β-d3-ol, β-methyl- (9CI) (CA INDEX NAME)



IT 849700-24-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of (R)-β-(methyl)benzenemethan-α,α-d2-ol by regioselective deuterium labeling using (phenyl)propanol and deuterium oxide as starting materials and dichlorobis(triphenylphosphine)ruthenium as catalyst)
RN 849700-24-9 CAPLUS
CN Benzeneethan-α,α-d2-ol, β-methyl-, (βR)- (9CI) (CA INDEX NAME)

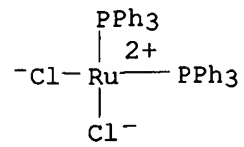
Absolute stereochemistry.



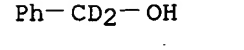
IT 849700-17-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of [(phenyl)methoxy]-1-decan-1,1-d2-ol by regioselective microwave-mediated deuterium labeling using primary alc. and deuterium oxide as starting materials and dichlorobis(triphenylphosphine)ruthenium as catalyst)
RN 849700-17-0 CAPLUS
CN 1-Decan-1,1-d2-ol, 10-(phenylmethoxy)- (9CI) (CA INDEX NAME)

$HO-CD_2-(CH_2)_9-O-CH_2-Ph$

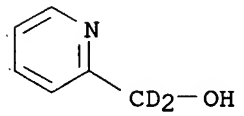
IT 34076-51-2, Dichlorobis(triphenylphosphine)ruthenium
RL: CAT (Catalyst use); USES (Uses)
(preparation of alkan-1,1-d2-ol and alkan-1,1-d2-amine derivs. by regioselective deuterium labeling using primary alcs. or amines and deuterium oxide as starting materials and dichlorobis(triphenylphosphine)ruthenium as catalyst)
RN 34076-51-2 CAPLUS
CN Ruthenium, dichlorobis(triphenylphosphine)- (CA INDEX NAME)



IT 21175-64-4P, Benzenemethan-d2-ol
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of benzenemethan-α,α-d2-ol by regioselective microwave-mediated deuterium labeling using primary alc. and deuterium oxide as starting materials and dichlorobis(triphenylphosphine)rutheniu m as catalyst)
RN 21175-64-4 CAPLUS
CN Benzenemethan-d2-ol (CA INDEX NAME)



IT 849700-16-9P, 2-Pyridinemethan-α,α-d2-ol
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of pyridinemethan-α,α-d2-ol by regioselective microwave-mediated deuterium labeling using primary alc. and deuterium oxide as starting materials and dichlorobis(triphenylphosphine)rutheniu m as catalyst)
RN 849700-16-9 CAPLUS
CN 2-Pyridinemethan-α,α-d2-ol (CA INDEX NAME)



REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

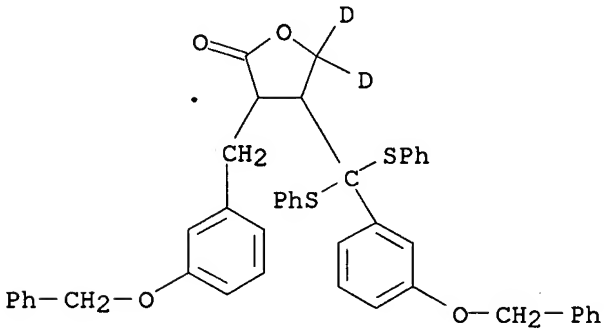
L24 ANSWER 19 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:859466 CAPLUS
DOCUMENT NUMBER: 143:97191
TITLE: Synthesis of deuterium labelled metabolites of plant lignans
AUTHOR(S): Leppala, Eija; Wahala, Kristiina
CORPORATE SOURCE: Department of Chemistry, Laboratory of Organic Chemistry, University of Helsinki, 00014, Finland
SOURCE: Synthesis and Applications of Isotopically Labelled Compounds, Proceedings of the International Symposium, 8th, Boston, MA, United States, June 1-5, 2003 (2004), Meeting Date 2003, 397-398. Editor(s): Dean, Dennis C.; Filer, Crist N.; McCarthy, Keith E. John Wiley & Sons Ltd.: Chichester, UK.
CODEN: 69FZAZ; ISBN: 0-470-86365-X
DOCUMENT TYPE: Conference
LANGUAGE: English
OTHER SOURCE(S): CASREACT 143:97191

AB In HPLC-MS or GC-MS, stable isotopic labeled lignans are needed as internal stds. to quantitate enterolignans in biol. samples. Butyrolactone type lignans can be synthesized by a tandem Michael addition-alkylation reaction followed by desulfurization and debenzylation with Raney nickel. An expedient deuterolabeling method for butyrolactone type lignans is the use of D3PO4BF3 in D2O. In the strongly acidic conditions all aromatic protons are changed to deuterium in good yield and with high isotopic purity. Diols can be formed from deuterated lactones by reduction with LiAlH4.

IT 856412-14-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(desulfurization and debenzylation of, with Raney nickel; synthesis of deuterium labeled metabolites of plant lignans)

RN 856412-14-1 CAPLUS

CN 2(3H)-Furanone-5-d, dihydro-5-d-4-[[3-(phenylmethoxy)phenyl]bis(phenylthio)methyl]-3-[[3-(phenylmethoxy)phenyl]methyl]- (9CI) (CA INDEX NAME)




IT 7440-02-0D, Nickel, Raney
RL: CAT (Catalyst use); USES (Uses)
(hydrogenolysis catalyst; synthesis of deuterium labeled metabolites of plant lignans)

RN 7440-02-0 CAPLUS

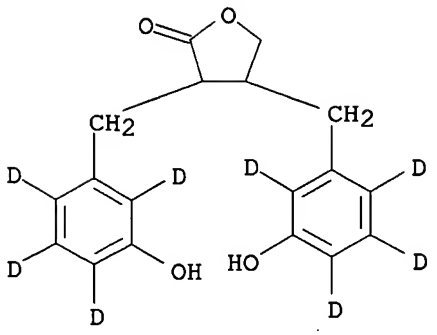
CN Nickel (CA INDEX NAME)

Ni

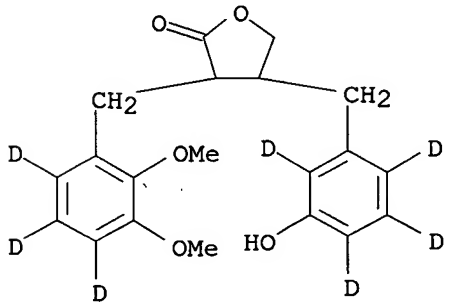
IT 856412-16-3P 856412-18-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and aluminohydride reduction of; synthesis of deuterium labeled metabolites of plant lignans)

RN 856412-16-3 CAPLUS

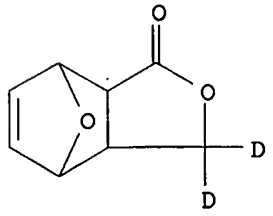
CN 2(3H)-Furanone, dihydro-3,4-bis[(5-hydroxyphenyl-2,3,4,6-d4)methyl]- (9CI) (CA INDEX NAME)



RN 856412-18-5 CAPLUS
CN 2(3H)-Furanone, 3-[(5,6-dimethoxyphenyl-2,3,4-d3)methyl]dihydro-4-[(5-hydroxyphenyl-2,3,4,6-d4)methyl]- (9CI) (CA INDEX NAME)

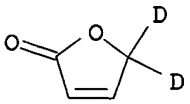


IT 96995-04-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and retro-Diels-Alder of; synthesis of deuterium labeled metabolites of plant lignans)
RN 96995-04-9 CAPLUS
CN 4,7-Epoxyisobenzofuran-1(3H)-one-3,3-d2, 3a,4,7,7a-tetrahydro- (9CI) (CA INDEX NAME)

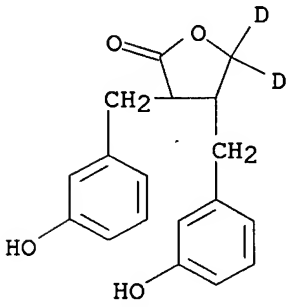


IT 53252-93-0P, 5,5-Dideutero-2,5-dihydro-2-furanone
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and tandem Michael addition-alkylation reaction of, with benzaldehyde thioacetals and benzyl bromides; synthesis of deuterium labeled metabolites of plant lignans)

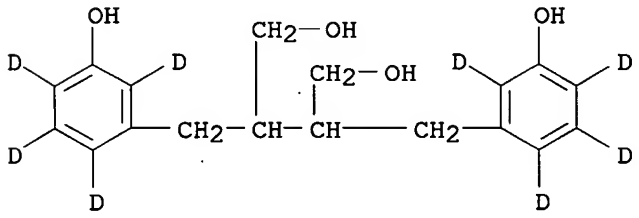
RN 53252-93-0 CAPLUS
CN 2(5H)-Furanone-5,5-d2 (9CI) (CA INDEX NAME)



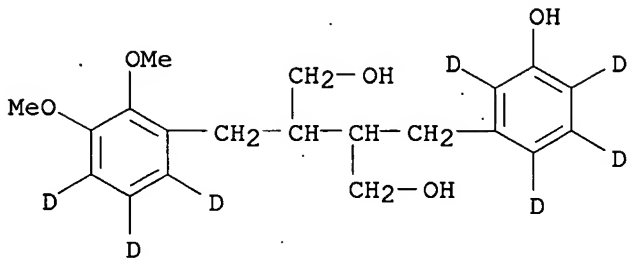
IT 856412-15-2P 856412-17-4P 856412-19-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of deuterium labeled metabolites of plant lignans)
RN 856412-15-2 CAPLUS
CN 2(3H)-Furanone-5-d, dihydro-5-d-3,4-bis[(3-hydroxyphenyl)methyl]- (9CI) (CA INDEX NAME)



RN 856412-17-4 CAPLUS
CN 1,4-Butanediol, 2,3-bis[(5-hydroxyphenyl-2,3,4,6-d4)methyl]- (9CI) (CA INDEX NAME)



RN 856412-19-6 CAPLUS
CN 1,4-Butanediol, 2-[(5,6-dimethoxyphenyl-2,3,4-d3)methyl]-3-[(5-hydroxyphenyl-2,3,4,6-d4)methyl]- (9CI) (CA INDEX NAME)



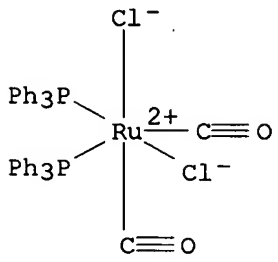
REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 20 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:800202 CAPLUS
DOCUMENT NUMBER: 141:424246
TITLE: Ruthenium-Catalyzed Hydrogenation of Alkynylstannanes with Migration of the Stannyl Group
AUTHOR(S): Shirakawa, Eiji; Morita, Ryotaro; Tsuchimoto, Teruhisa; Kawakami, Yusuke
CORPORATE SOURCE: Department of Chemistry, Graduate School of Science, Kyoto University, Kyoto, 606-8502, Japan
SOURCE: Journal of the American Chemical Society (2004), 126(42), 13614-13615
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 141:424246

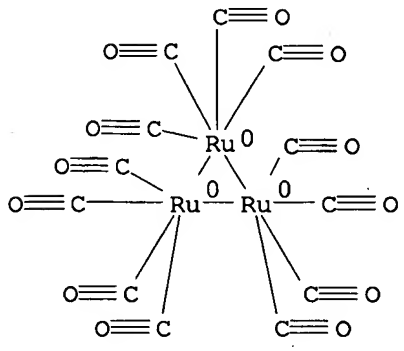
AB Mol. hydrogen adds to aliphatic and aromatic alkynylstannanes in the presence of a ruthenium catalyst, pushing the stannyl group to the adjacent carbon atom to give α-substituted vinylstannanes. For example, CH3(CH2)5C.tplbond.CSnBu3 reacted with H2 in the presence of RuH2(CO)(PPh3)3 and PBu3 giving CH3(CH2)5C(SnBu3):CH2 in 92% yield. This is the first achievement of hydrogenation of alkynylstannanes, which is applicable also to the deuteration affording precursors for an important class of deuterium-labeled compds.

IT 14564-35-3 15243-33-1, Dodecacarbonyltriruthenium
25360-32-1 41290-68-0 52462-29-0
794535-47-0
RL: CAT (Catalyst use); USES (Uses)
(preparation of vinylstannanes via ruthenium-catalyzed hydrogenation of alkynylstannanes with migration of the stannyl group)

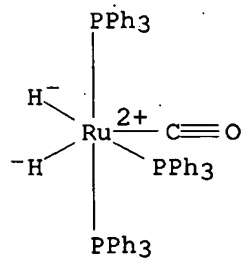
RN 14564-35-3 CAPLUS
CN Ruthenium, dicarbonyldichlorobis(triphenylphosphine)- (CA INDEX NAME)



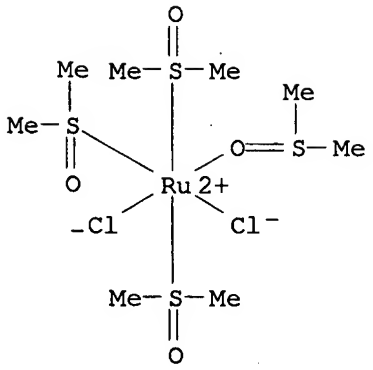
RN 15243-33-1 CAPLUS
CN Ruthenium, dodecacarbonyltri-, triangulo (CA INDEX NAME)



RN 25360-32-1 CAPLUS
CN Ruthenium, carbonyldihydrotris(triphenylphosphine)- (CA INDEX NAME)

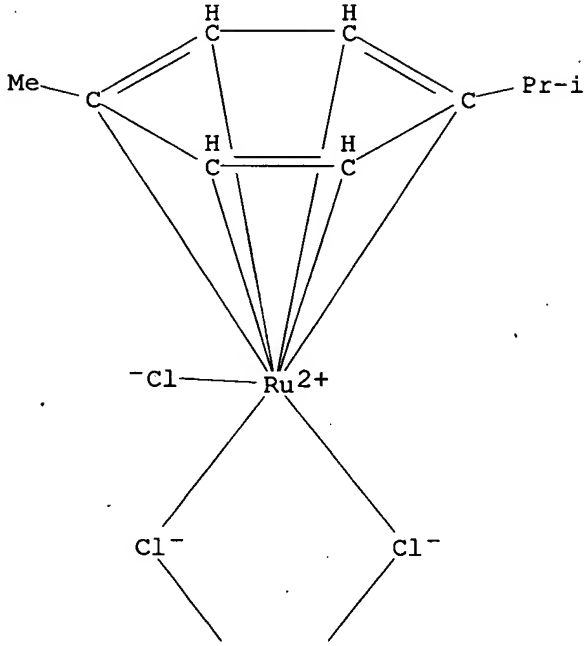


RN 41290-68-0 CAPLUS
CN Ruthenium, dichloro[1,1'-(sulfinyl-κO)bis[methane]]tris[1,1'-(sulfinyl-κS)bis[methane]]- (CA INDEX NAME)

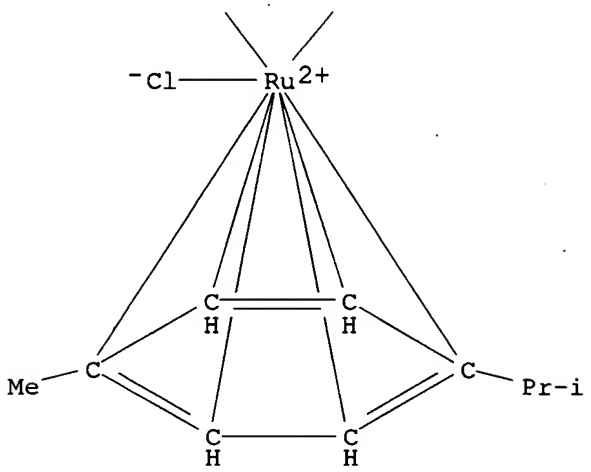


RN 52462-29-0 CAPLUS
CN Ruthenium, di-μ-chlorodichlorobis[(1,2,3,4,5,6-η)-1-methyl-4-(1-methylethyl)benzene]di- (CA INDEX NAME)

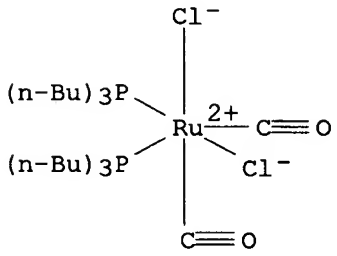
PAGE 1-A



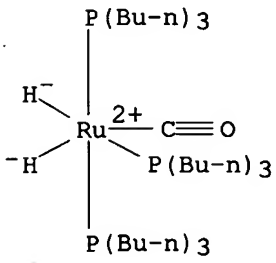
PAGE 2-A




RN 794535-47-0 CAPLUS
CN Ruthenium, dicarbonyldichlorobis(tributylphosphine)- (CA INDEX NAME)

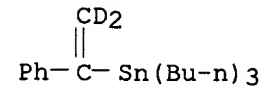



IT 149006-06-4P
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation of vinylstannanes via ruthenium-catalyzed hydrogenation of alkynylstannanes with migration of the stannyl group)
RN 149006-06-4 CAPLUS
CN Ruthenium, carbonyldihydrotris(tributylphosphine)- (CA INDEX NAME)

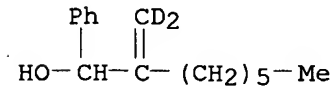



IT 793719-94-5P 793719-96-7P 793719-98-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of vinylstannanes via ruthenium-catalyzed hydrogenation of

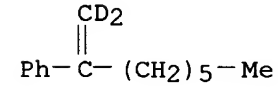
alkynylstannanes with migration of the stannyl group)
RN 793719-94-5 CAPLUS
CN Stannane, tributyl(1-phenylethenyl-2,2-d2)- (9CI) (CA INDEX NAME)



RN 793719-96-7 CAPLUS
CN Benzenemethanol, α-[1-(methylene-d2)heptyl]- (9CI) (CA INDEX NAME)



RN 793719-98-9 CAPLUS
CN Benzene, [1-(methylene-d2)heptyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 21 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:589514 CAPLUS
DOCUMENT NUMBER: 141:139883
TITLE: Method of catalytic deuteration of carbonyl compounds or secondary alcohols by heavy water
INVENTOR(S): Ito, Nobuhiro; Maesawa, Tsuneaki; Muto, Kazushige; Hirota, Kosaku; Sajiki, Hironao
PATENT ASSIGNEE(S): Wako Pure Chemical Industries, Ltd., Japan
SOURCE: PCT Int. Appl., 42 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2004060831 | A1 | 20040722 | WO 2003-JP14182 | 20031107 |

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,

BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

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|---|---|---|---|---|
| CA 2511885 | A1 | 20040722 | CA 2003-2511885 | 20031107 |
| AU 2003277596 | A1 | 20040729 | AU 2003-277596 | 20031107 |
| EP 1577280 | A1 | 20050921 | EP 2003-814536 | 20031107 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK | | | | |
| CN 1732135 | A | 20060208 | CN 2003-80107483 | 20031107 |
| US 20060116535 | A1 | 20060601 | US 2005-539188 | 20050616 |
| IN 2005KN01449 | A | 20070720 | IN 2005-KN1449 | 20050726 |
| PRIORITY APPLN. INFO.: | | | JP 2002-378932 A | 20021227 |
| | | | WO 2003-JP14182 W | 20031107 |

OTHER SOURCE(S): CASREACT 141:139883; MARPAT 141:139883

AB Described is a method of deuterating a carbonyl or secondary alc. compound represented by the general formula R1-X-R2 (I) (wherein R1 = alkyl optionally possessing a CH:CH or C.tplbond.C bond, aralkyl ; R2 = alkyl optionally possessing a CH:CH or C.tplbond.C bond, aryl, aralkyl, alkoxy, aryloxy, hydroxy; X carbonyl, hydroxymethylene), which comprises reacting the compound represented by the general formula I with a deuterium source, in particular D2O, in the presence of a catalyst selected among activated palladium, platinum, rhodium, ruthenium, nickel, and cobalt catalysts. By the method, deuteration, which has been conducted under severe conditions, can be conducted under neutral conditions. Even when the compound contains an unsatd. bond, it can be deuterated without reducing the unsatd. bond. Not only hydrogens near the carbonyl or hydroxymethylene group but also those remotely situated from these groups are selectively deuterated without deuterating the carbon-carbon double or triple bonds. Thus, 500 mg tricyclo[5.2.1.02'6]decan-8-ol and 100 mg Pd-C were suspended in 17 mL D2O, purged with H, and heated at 180° for 24 h in an oil bath to give tricyclo[5.2.1.02'6]decan-8-ol deuterated by 96% at 8-position and 88% at other positions.

IT 7440-02-0, Raney nickel, uses
RL: CAT (Catalyst use); USES (Uses)
(catalysts; catalytic deuteration of carbonyl compds. or secondary alc. compds. with heavy water in presence of palladium, platinum, rhodium, ruthenium, or nickel)

RN 7440-02-0 CAPLUS

CN Nickel (CA INDEX NAME)

Ni

IT 7440-06-4, Platinum, uses 7440-06-4D, Platinum, supported on carbon 7440-16-6, Rhodium, uses 7440-16-6D , Rhodium, supported on alumina 7440-18-8, Ruthenium, uses 7440-18-8D, Ruthenium, supported on carbon 7440-48-4, Cobalt, uses
RL: CAT (Catalyst use); USES (Uses)
(catalytic deuteration of carbonyl compds. or secondary alc. compds. with heavy water in presence of palladium, platinum, rhodium, ruthenium, or nickel)

RN 7440-06-4 CAPLUS

CN Platinum (CA INDEX NAME)

Pt

RN 7440-06-4 CAPLUS
CN Platinum (CA INDEX NAME)

Pt

RN 7440-16-6 CAPLUS
CN Rhodium (CA INDEX NAME)

Rh

RN 7440-16-6 CAPLUS
CN Rhodium (CA INDEX NAME)

Rh

RN 7440-18-8 CAPLUS
CN Ruthenium (CA INDEX NAME)

Ru

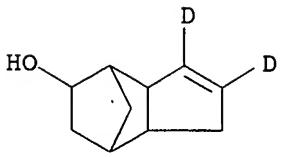
RN 7440-18-8 CAPLUS
CN Ruthenium (CA INDEX NAME)

Ru

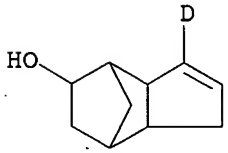
RN 7440-48-4 CAPLUS
CN Cobalt (CA INDEX NAME)

Co

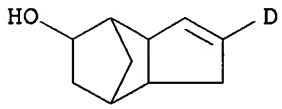
IT 725242-26-2DP, deuterated 725242-27-3DP, deuterated
725242-28-4DP, deuterated
RL: SPN (Synthetic preparation); PREP (Preparation)
(catalytic deuteration of carbonyl compds. or secondary alc. compds. with heavy water in presence of palladium, platinum, rhodium, ruthenium, or nickel)
RN 725242-26-2 CAPLUS
CN 4,7-Methano-1H-inden-2,3-d2-5-ol, 3a,4,5,6,7,7a-hexahydro- (9CI) (CA INDEX NAME)



RN 725242-27-3 CAPLUS
CN 4,7-Methano-1H-inden-3-d-5-ol, 3a,4,5,6,7,7a-hexahydro- (9CI) (CA INDEX NAME)



RN 725242-28-4 CAPLUS
CN 4,7-Methano-1H-inden-2-d-5-ol, 3a,4,5,6,7,7a-hexahydro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 22 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:453150 CAPLUS
DOCUMENT NUMBER: 141:23545
TITLE: Method for deuteration or tritiation of heterocyclic compounds
INVENTOR(S): Ito, Nobuhiro; Maesawa, Tsuneaki; Muto, Kazushige; Hirota, Kosaku; Sajiki, Hironao
PATENT ASSIGNEE(S): Wako Pure Chemical Industries, Ltd., Japan
SOURCE: PCT Int. Appl., 45 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2004046066 | A1 | 20040603 | WO 2003-JP14181 | 20031107 |

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

| | | | | |
|---|---|---|---|---|
| CA 2506010 | A1 | 20040603 | CA 2003-2506010 | 20031107 |
| AU 2003277595 | A1 | 20040615 | AU 2003-277595 | 20031107 |
| EP 1561741 | A1 | 20050810 | EP 2003-811499 | 20031107 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK | | | | |
| CN 1714060 | A | 20051228 | CN 2003-80103924 | 20031107 |
| US 20060025596 | A1 | 20060202 | US 2005-534344 | 20050509 |
| IN 2005KN01145 | A | 20061110 | IN 2005-KN1145 | 20050615 |
| PRIORITY APPLN. INFO.: | | | JP 2002-331594 A | 20021115 |
| | | | WO 2003-JP14181 W | 20031107 |

AB A method for deuteration or tritiation of a heterocyclic ring comprises allowing a heterocyclic compound to be present under a sealing and refluxing condition in a deuterated or tritiated solvent (e.g., D2O) in the presence of an activated catalyst selected from among a palladium catalyst, a platinum catalyst, a rhodium catalyst, a ruthenium catalyst, a nickel catalyst and a cobalt catalyst. The method allows a deuteration or tritiation temperature to be kept at a temperature higher than the boiling temperature of the solvent, which results in the replacement of a hydrogen atom in a heterocyclic ring of a heterocyclic compound with very good efficiency. Further, the method can be widely used for the deuteration or tritiation of various types of heterocyclic compds. in a com. process.

IT 7440-02-0, Nickel, uses 7440-06-4, Platinum, uses 7440-16-6, Rhodium, uses 7440-18-8, Ruthenium, uses 7440-48-4, Cobalt, uses
RL: CAT (Catalyst use); USES (Uses)
(method for deuteration or tritiation of heterocyclic compds.)

RN 7440-02-0 CAPLUS
CN Nickel (CA INDEX NAME)

Ni

RN 7440-06-4 CAPLUS
CN Platinum (CA INDEX NAME)

Pt

RN 7440-16-6 CAPLUS
CN Rhodium (CA INDEX NAME)

Rh

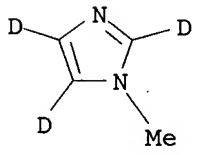
RN 7440-18-8 CAPLUS
CN Ruthenium (CA INDEX NAME)

Ru

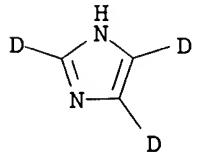
RN 7440-48-4 CAPLUS
CN Cobalt (CA INDEX NAME)

Co

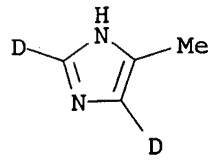
IT 4166-68-1P 6745-43-3P, 1H-Imidazole-2,4,5-d3
22194-79-2P 24897-52-7P, 2,4(1H,3H)-Pyrimidinedione-5,6-d2 40632-21-1P, Uridine-5,6-d2 62595-11-3P, L-Tryptophan-2,4,5,6,7-d5 82845-88-3P, Adenosine-2,8-d2 96412-41-8P, Guanosine-8-d 106391-24-6P 130317-91-8P 200496-79-3P 350818-65-4P 697806-98-7P 697806-99-8P 697807-00-4P, 1H-Purin-2,8-d2-6-amine 697807-01-5P, Inosine-2,8-d2 697807-02-6P 697807-03-7P 697807-04-8P 697807-05-9P 697807-06-0P 697807-07-1P
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(method for deuteration or tritiation of heterocyclic compds.)
RN 4166-68-1 CAPLUS
CN 1H-Imidazole-2,4,5-d3, 1-methyl- (9CI) (CA INDEX NAME)



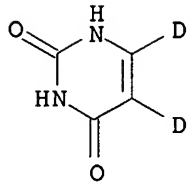
RN 6745-43-3 CAPLUS
CN 1H-Imidazole-2,4,5-d3 (9CI) (CA INDEX NAME)



RN 22194-79-2 CAPLUS
CN 1H-Imidazole-2,4-d2, 5-methyl- (9CI) (CA INDEX NAME)

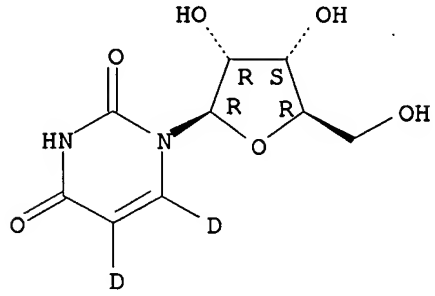


RN 24897-52-7 CAPLUS
CN 2,4(1H,3H)-Pyrimidinedione-5,6-d2 (CA INDEX NAME)



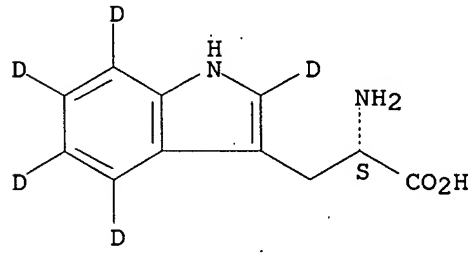
RN 40632-21-1 CAPLUS
CN Uridine-5,6-d2 (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



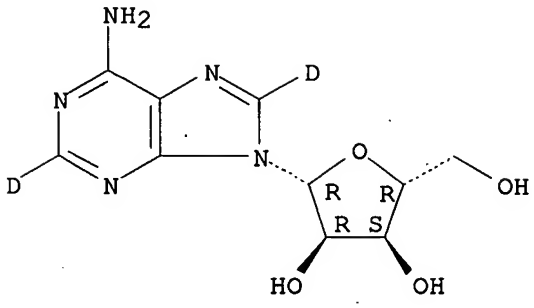
RN 62595-11-3 CAPLUS
CN L-Tryptophan-2,4,5,6,7-d5 (9CI) (CA INDEX NAME)

Absolute stereochemistry.



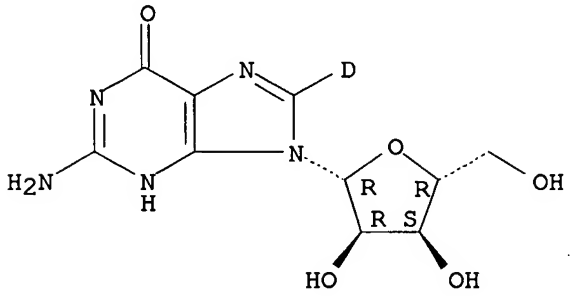
RN 82845-88-3 CAPLUS
CN Adenosine-2,8-d2 (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

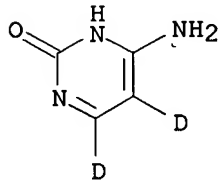


RN 96412-41-8 CAPLUS
CN Guanosine-8-d (9CI) (CA INDEX NAME)

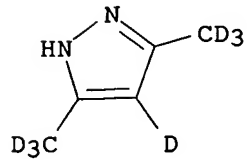
Absolute stereochemistry. Rotation (-).



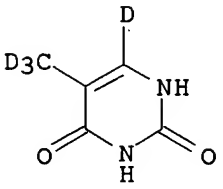
RN 106391-24-6 CAPLUS
CN 2(1H)-Pyrimidinone-4,5-d2, 6-amino- (9CI) (CA INDEX NAME)



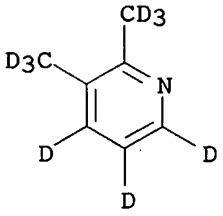
RN 130317-91-8 CAPLUS
CN 1H-Pyrazole-4-d, 3,5-di(methyl-d3)- (CA INDEX NAME)



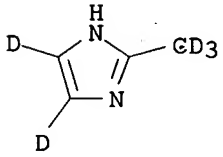
RN 200496-79-3 CAPLUS
CN 2,4(1H,3H)-Pyrimidinedione-6-d, 5-(methyl-d3)- (CA INDEX NAME)



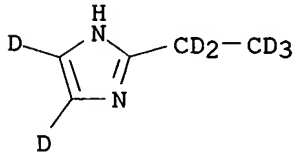
RN 350818-65-4 CAPLUS
CN Pyridine-2,3,4-d3, 5,6-di(methyl-d3)- (9CI) (CA INDEX NAME)



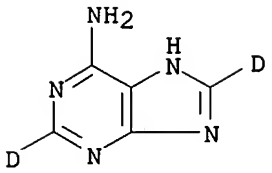
RN 697806-98-7 CAPLUS
CN 1H-Imidazole-4,5-d2, 2-(methyl-d3)- (9CI) (CA INDEX NAME)



RN 697806-99-8 CAPLUS
CN 1H-Imidazole-4,5-d2, 2-(ethyl-d5)- (9CI) (CA INDEX NAME)

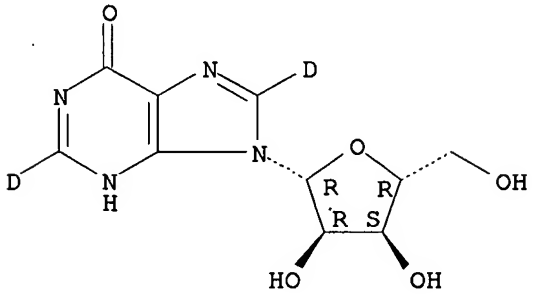


RN 697807-00-4 CAPLUS
CN 1H-Purin-2,8-d2-6-amine (9CI) (CA INDEX NAME)

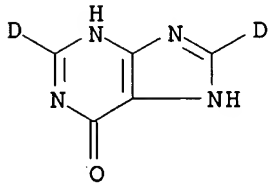


RN 697807-01-5 CAPLUS
CN Inosine-2,8-d2 (9CI) (CA INDEX NAME)

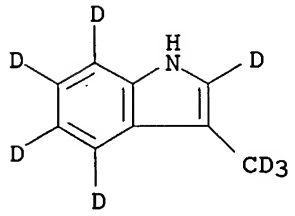
Absolute stereochemistry. Rotation (-).



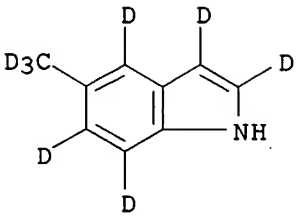
RN 697807-02-6 CAPLUS
CN 6H-Purin-6-one-2,8-d2, 1,7-dihydro- (9CI) (CA INDEX NAME)



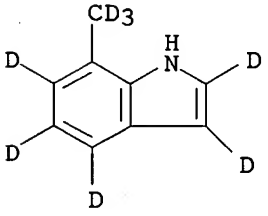
RN 697807-03-7 CAPLUS
CN 1H-Indole-2,4,5,6,7-d5, 3-(methyl-d3)- (CA INDEX NAME)



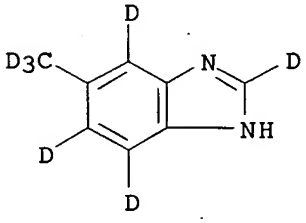
RN 697807-04-8 CAPLUS
CN 1H-Indole-2,3,4,6,7-d5, 5-(methyl-d3)- (9CI) (CA INDEX NAME)



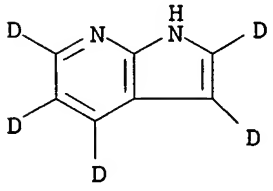
RN 697807-05-9 CAPLUS
CN 1H-Indole-2,3,4,5,6-d5, 7-(methyl-d3)- (CA INDEX NAME)



RN 697807-06-0 CAPLUS
CN 1H-Benzimidazole-2,4,5,7-d4, 6-(methyl-d3)- (CA INDEX NAME)



RN 697807-07-1 CAPLUS
CN 1H-Pyrrolo[2,3-b]pyridine-2,3,4,5,6-d5 (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 23 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:101109 CAPLUS
DOCUMENT NUMBER: 140:163571

TITLE: Process for preparation of deuterated aromatic compounds
INVENTOR(S): Ito, Nobuhiro; Maesawa, Tsuneaki; Muto, Kazushige; Hirota, Kosaku; Sajiki, Hironao
PATENT ASSIGNEE(S): Wako Pure Chemical Industries, Ltd., Japan
SOURCE: PCT Int. Appl., 43 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| WO 2004011400 | A1 | 20040205 | WO 2003-JP8783 | 20030710 |
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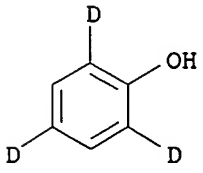
| RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG | | | | |
| CA 2493773 | A1 | 20040205 | CA 2003-2493773 | 20030710 |
| AU 2003248267 | A1 | 20040216 | AU 2003-248267 | 20030710 |
| EP 1535889 | A1 | 20050601 | EP 2003-771263 | 20030710 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK | | | | |
| CN 1675145 | A | 20050928 | CN 2003-818820 | 20030710 |
| US 20070255076 | A1 | 20071101 | US 2007-521531 | 20070222 |
| PRIORITY APPLN. INFO.: | | | JP 2002-219005 A | 20020726 |
| | | | WO 2003-JP8783 W | 20030710 |

AB This invention pertains to a method for deuterating a compound having an aromatic ring in the presence of an activated catalyst. For example, phenol was treated with D2O in the presence of Pt/C to give C6D5OH in 98% deuterating rate. This invention provides a method to make deuterated aromatic compds. in mild conditions.

IT 7329-50-2P, Phen-2,4,6-d3-ol
RL: BYP (Byproduct); PREP (Preparation)
(preparation of deuterated aromatic compds.)
RN 7329-50-2 CAPLUS
CN Phen-2,4,6-d3-ol (CA INDEX NAME)




IT 7440-02-0, Nickel, uses 7440-06-4, Platinum, uses 7440-16-6, Rhodium, uses 7440-18-8, Ruthenium, uses 7440-48-4, Cobalt, uses 10025-99-7, Platinous potassium chloride

RL: CAT (Catalyst use); USES (Uses)
(preparation of deuterated aromatic compds.)
RN 7440-02-0 CAPLUS
CN Nickel (CA INDEX NAME)

Ni

RN 7440-06-4 CAPLUS
CN Platinum (CA INDEX NAME)

Pt

RN 7440-16-6 CAPLUS
CN Rhodium (CA INDEX NAME)

Rh

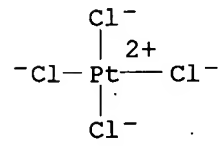
RN 7440-18-8 CAPLUS
CN Ruthenium (CA INDEX NAME)

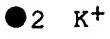
Ru

RN 7440-48-4 CAPLUS
CN Cobalt (CA INDEX NAME)

Co

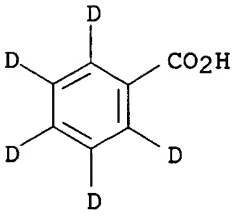
RN 10025-99-7 CAPLUS
CN Platinate(2-), tetrachloro-, potassium (1:2), (SP-4-1)- (CA INDEX NAME)



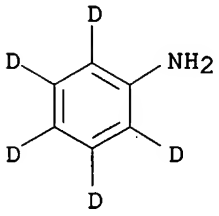


IT 1079-02-3P, Benzoic-d5 acid 4165-61-1P, Benzen-d5-amine
4165-62-2P, Phen-d5-ol 35782-14-0P 62790-26-5P
74383-28-1DP, deuterated 87976-31-6DP, Benzoic-3,4,5-d3
acid, deuterated 291765-93-0P, 1,2-Benzene-3,4,5,6-d4-diamine
654062-93-8P
RL: SPN (Synthetic preparation); PREP (Preparation)

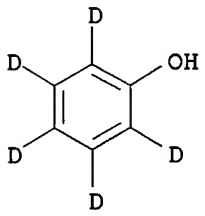
(preparation of deuterated aromatic compds.)
RN 1079-02-3 CAPLUS
CN Benzoic-2,3,4,5,6-d5 acid (CA INDEX NAME)



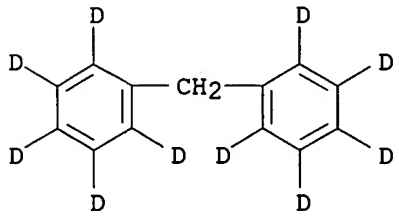
RN 4165-61-1 CAPLUS
CN Benzen-2,3,4,5,6-d5-amine (CA INDEX NAME)



RN 4165-62-2 CAPLUS
CN Phen-2,3,4,5,6-d5-ol (CA INDEX NAME)

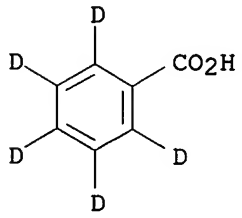


RN 35782-14-0 CAPLUS
CN Benzene-d5, 6,6'-methylenebis- (9CI) (CA INDEX NAME)



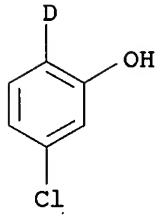
RN 62790-26-5 CAPLUS

CN Benzoic-d5 acid, sodium salt (9CI) (CA INDEX NAME)

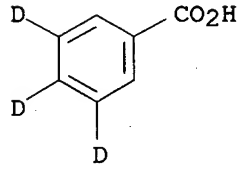


● Na

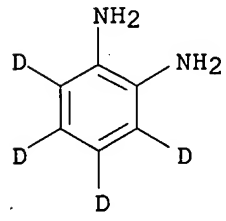
RN 74383-28-1 CAPLUS
CN Phen-2-d-ol, 5-chloro- (9CI) (CA INDEX NAME)



RN 87976-31-6 CAPLUS
CN Benzoic-3,4,5-d3 acid (9CI) (CA INDEX NAME)

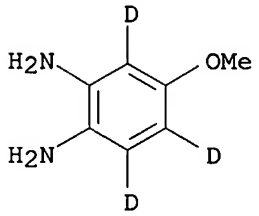


RN 291765-93-0 CAPLUS
CN 1,2-Benzene-3,4,5,6-d4-diamine (9CI) (CA INDEX NAME)



RN 654062-93-8 CAPLUS

CN 1,2-Benzene-3,4,6-d3-diamine, 5-methoxy- (9CI) (CA INDEX NAME)

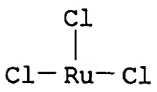


REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 24 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:900375 CAPLUS
DOCUMENT NUMBER: 140:128633
TITLE: A new synthesis of enantiomerically pure α- and β-amino acid derivatives using aziridinyl anions
AUTHOR(S): Satoh, Tsuyoshi; Fukuda, Yuta
CORPORATE SOURCE: Department of Chemistry, Faculty of Science, Tokyo University of Science, Kagurazaka, Shinjuku-ku, Tokyo, 162-8601, Japan
SOURCE: Tetrahedron (2003), 59(49), 9803-9810
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:128633

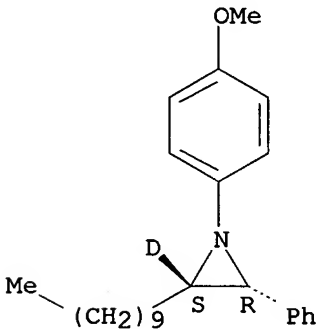
AB Optically active sulfinylaziridines having a 4-methoxyphenyl group on their nitrogen atom were synthesized from optically active 1-chloroalkyl p-tolyl sulfoxide and an imine derived from benzaldehyde and p-anisidine stereoselectively in good overall yields. The sulfinylaziridines were treated with ethylmagnesium bromide or tert-butyllithium to afford aziridinylmagnesiums or aziridinyllithiums, resp., in quant. yields. Cross-coupling of the aziridinylmagnesiums with iodoalkanes in the presence of Cu(I) iodide gave tri-substituted aziridines in high yields from which enantiomerically pure β,β-disubstituted β-amino acid derivs. were synthesized. A β-amino acid derivative having deuterium at the stereogenic center was also realized by this method. On the other hand, from the aziridinyllithium, enantiomerically pure quaternary phenylalanine and quaternary aspartic acid derivs. were synthesized.

IT 14898-67-0, Ruthenium trichloride hydrate
RL: CAT (Catalyst use); USES (Uses)
(preparation of enantiomerically pure α- and β-amino acid derivs. using aziridinyl anions)
RN 14898-67-0 CAPLUS
CN Ruthenium chloride (RuCl3), hydrate (8CI, 9CI) (CA INDEX NAME)



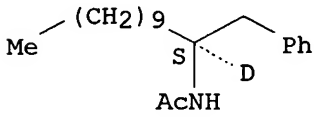
IT 648908-38-7P 648908-41-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of enantiomerically pure α- and β-amino acid derivs. using aziridinyl anions)
RN 648908-38-7 CAPLUS
CN Aziridine-2-d, 2-decyl-1-(4-methoxyphenyl)-3-phenyl-, (2S,3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 648908-41-2 CAPLUS
CN Acetamide, N-[(1S)-1-(phenylmethyl)undecyl-1-d]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

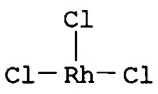
L24 ANSWER 25 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:474175 CAPLUS
DOCUMENT NUMBER: 139:395665
TITLE: Combining microwave-enhanced deuteration reactions with parallel synthesis procedures
AUTHOR(S): Chappelle, Michael R.; Harding, John R.; Kent, Barry B.; Jones, John R.; Lu, Shui-Yu; Morgan, Alan D.
CORPORATE SOURCE: Amersham Biosciences, The Maynard Centre, Cardiff, CF14 7YT, UK

SOURCE: Journal of Labelled Compounds & Radiopharmaceuticals (2003), 46(6), 567-574
CODEN: JLCRD4; ISSN: 0362-4803
PUBLISHER: John Wiley & Sons Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:395665

AB The development of combined microwave-enhanced/parallel synthesis procedures and their application to the deuteration of organic compds. via examples of solid-state hydrogenation is reported. Other labeling procedures, such as solution state catalytic dehalogenations, hydrogenations as well as hydrogen isotope exchange reactions also benefit from the combined technol.

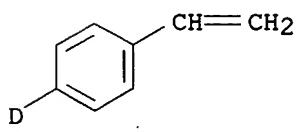
IT 10049-07-7, Rhodium chloride (RhCl3)
RL: CAT (Catalyst use); USES (Uses)
(combining microwave-enhanced deuteration with parallel synthesis procedures)

RN 10049-07-7 CAPLUS
CN Rhodium chloride (RhCl3) (CA INDEX NAME)

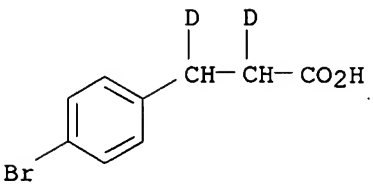


IT 10473-16-2P 625383-68-8P, 4-Bromobenzenepropanoic-α,β-d2 acid potassium salt 625383-69-9P, 3-(Phenyl-4-d)-2-Propenoic acid potassium salt 625383-72-4P 625383-73-5P, 3-(Phenyl-3-d)-2-Propenoic acid potassium salt 625383-74-6P, 1-Bromo-4-(ethyl-1,2-d2)benzene 625383-78-0P 625383-80-4P, 4-Fluorobenzenepropanoic-α,β-d2 acid potassium salt 625383-82-6P, 2-Chlorobenzenepropanoic-α,β-d2 acid potassium salt 625383-84-8P, 3-Chlorobenzenepropanoic-α,β-d2 acid potassium salt 625383-86-0P, 4-Chlorobenzenepropanoic-α,β-d2 acid potassium salt 625383-88-2P, 1-Bromo-4-(ethenyl-1,2-d2)benzene 625383-90-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(combining microwave-enhanced deuteration with parallel synthesis procedures)

RN 10473-16-2 CAPLUS
CN Benzene-d, 4-ethenyl- (9CI) (CA INDEX NAME)

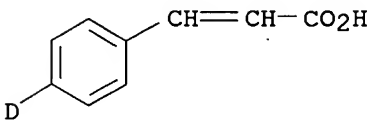


RN 625383-68-8 CAPLUS
CN Benzenepropanoic-α,β-d2 acid, 4-bromo-, potassium salt (9CI) (CA INDEX NAME)



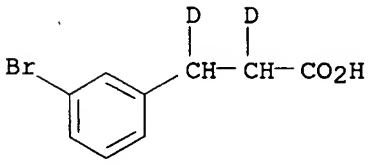
● K

RN 625383-69-9 CAPLUS
CN 2-Propenoic acid, 3-(phenyl-4-d)-, potassium salt (9CI) (CA INDEX NAME)



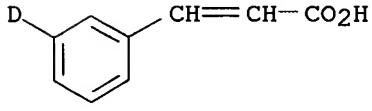
● K

RN 625383-72-4 CAPLUS
CN Benzenepropanoic-α,β-d2 acid, 3-bromo-, potassium salt (9CI) (CA INDEX NAME)



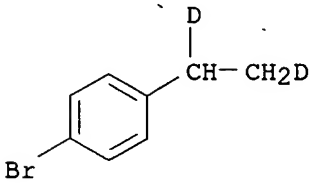
● K

RN 625383-73-5 CAPLUS
CN 2-Propenoic acid, 3-(phenyl-3-d)-, potassium salt (9CI) (CA INDEX NAME)

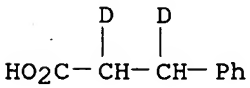


● K

RN 625383-74-6 CAPLUS
CN Benzene, 1-bromo-4-(ethyl-1,2-d2)- (9CI) (CA INDEX NAME)

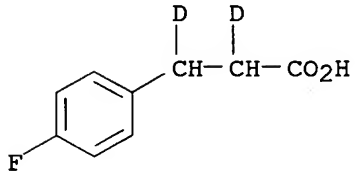


RN 625383-78-0 CAPLUS
CN Benzenepropanoic-α,β-d2 acid, potassium salt (9CI) (CA INDEX NAME)



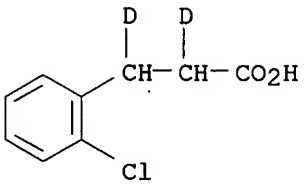
● K

RN 625383-80-4 CAPLUS
CN Benzenepropanoic-α,β-d2 acid, 4-fluoro-, potassium salt (9CI) (CA INDEX NAME)



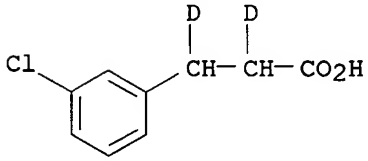
● K

RN 625383-82-6 CAPLUS
CN Benzenepropanoic-α,β-d2 acid, 2-chloro-, potassium salt (9CI) (CA INDEX NAME)



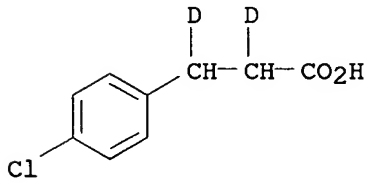
● K

RN 625383-84-8 CAPLUS
CN Benzenepropanoic-α,β-d2 acid, 3-chloro-, potassium salt (9CI) (CA INDEX NAME)



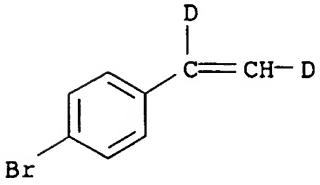
● K

RN 625383-86-0 CAPLUS
CN Benzenepropanoic-α,β-d2 acid, 4-chloro-, potassium salt (9CI) (CA INDEX NAME)

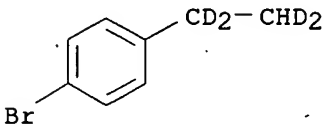


● K

RN 625383-88-2 CAPLUS
CN Benzene, 1-bromo-4-(ethenyl-1,2-d2)- (9CI) (CA INDEX NAME)

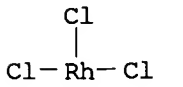


RN 625383-90-6 CAPLUS
CN Benzene, 1-bromo-4-(ethyl-1,1,2,2-d4)- (9CI) (CA INDEX NAME)

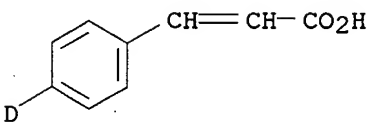



REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

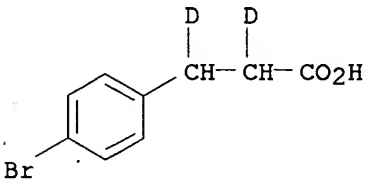
L24 ANSWER 26 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2002:483457 CAPLUS
DOCUMENT NUMBER: 138:4188
TITLE: Development of combined microwave-enhanced labelling procedures for maximizing deuterium incorporation
AUTHOR(S): Chapelle, Michael R.; Kent, Barry B.; Jones, John R.; Lu, Shui-Yu; Morgan, Alan D.
CORPORATE SOURCE: Amersham Plc, Cardiff Laboratories, Cardiff, CF14 7YT, UK
SOURCE: Tetrahedron Letters (2002), 43(29), 5117-5118
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:4188
AB Combined hydrogenation/aromatic dehalogenation under microwave-enhanced conditions provides a rapid route to deuterium labeled compds. with enhanced isotopic incorporation.
IT 10049-07-7, Rhodium chloride (RhCl3)
RL: CAT (Catalyst use); USES (Uses)
(microwave-induced rhodium- and palladium-catalyzed combined hydrogenation/aromatic dehalogenation routes for preparation of deuterium-labeled compds. with enhanced isotopic incorporation)
RN 10049-07-7 CAPLUS
CN Rhodium chloride (RhCl3) (CA INDEX NAME)



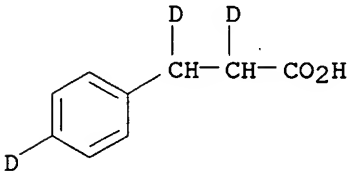

IT 99532-30-6P 477284-15-4P 477284-16-5P,
Benzene-4-d-propanoic-α,β-d2 acid
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of deuterium-labeled compds. with enhanced isotopic incorporation via combined microwave-induced hydrogenation/aromatic dehalogenation procedure)
RN 99532-30-6 CAPLUS
CN 2-Propenoic acid, 3-(phenyl-4-d)- (9CI) (CA INDEX NAME)



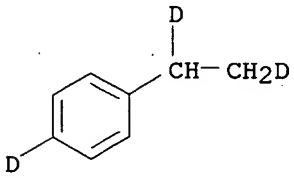
RN 477284-15-4 CAPLUS
CN Benzenepropanoic-α,β-d2 acid, 4-bromo- (9CI) (CA INDEX NAME)



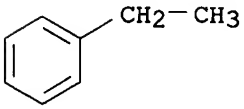
RN 477284-16-5 CAPLUS
CN Benzene-4-d-propanoic-α,β-d2 acid (9CI) (CA INDEX NAME)



IT 477284-18-7P 477284-19-8P, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of deuterium-labeled compds. with enhanced isotopic incorporation via microwave-induced dehalogenation procedure)
RN 477284-18-7 CAPLUS
CN Benzene-d, 4-(ethyl-1,2-d2)- (9CI) (CA INDEX NAME)



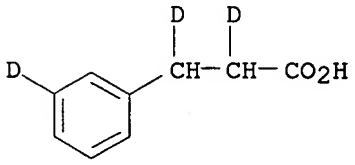
RN 477284-19-8 CAPLUS
CN Benzene, ethyl-, labeled with deuterium (9CI) (CA INDEX NAME)



IT 477284-17-6P, Benzene-3-d-propanoic-α,β-d2 acid

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of deuterium-labeled compds. with enhanced isotopic incorporation via microwave-induced hydrogenation/aromatic dehalogenation procedure)

RN 477284-17-6 CAPLUS
CN Benzene-3-d-propanoic-α,β-d2 acid (9CI) (CA INDEX NAME)



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 27 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2001:862887 CAPLUS
DOCUMENT NUMBER: 136:262857
TITLE: Hydrogenation of quinoline by rhodium catalysts modified with the tripodal polyphosphine ligand MeC(CH2PPh2)3
AUTHOR(S): Bianchini, Claudio; Barbaro, Pierluigi; Macchi, Michela; Meli, Andrea; Vizza, Francesco
CORPORATE SOURCE: Istituto per lo Studio della Stereochimica ed Energetica dei Composti di Coordinazione, ISSECC-CNR, Florence, I-50132, Italy
SOURCE: Helvetica Chimica Acta (2001), 84(10), 2895-2923
CODEN: HCACAV; ISSN: 0018-019X
PUBLISHER: Verlag Helvetica Chimica Acta
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 136:262857

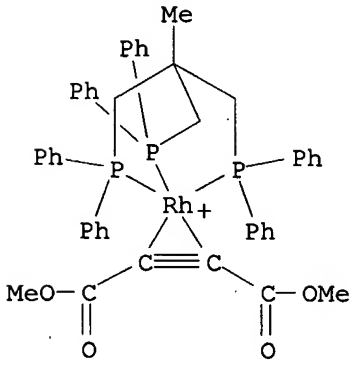
AB As part of our modeling studies of the hydrodenitrogenation of N-heterocycles contained in raw oil materials, we investigated the selective hydrogenation of quinoline to 1,2,3,4-tetrahydroquinoline by rhodium catalysts modified with the tripodal polyphosphane ligand MeC(CH2PPh2)3. Expts. in standard autoclaves and in high-pressure sapphire NMR tubes, kinetic and isotope labeling studies, and independent reactions with isolated compds. have contributed to the elucidation of the catalytic mechanism as well as identification of the electronic requisites of the metal catalyst for selective and efficient hydrogenation.

IT 182065-81-2
RL: CAT (Catalyst use); CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent); USES (Uses)
(Hydrogenation of quinoline by rhodium catalysts modified with the tripodal polyphosphine ligand MeC(CH2PPh2)3)

RN 182065-81-2 CAPLUS
CN Rhodium(1+), [(2,3-η)-dimethyl 2-butynedioate][[2-[(diphenylphosphino-κP)methyl]-2-methyl-1,3-propanediyl]bis[diphenylphosphine-κP]]-, hexafluorophosphate(1-) (9CI) (CA INDEX NAME)

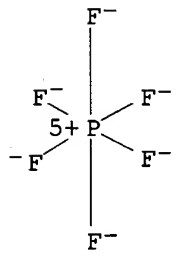
CM 1

CRN 116863-73-1
CMF C47 H45 O4 P3 Rh
CCI CCS

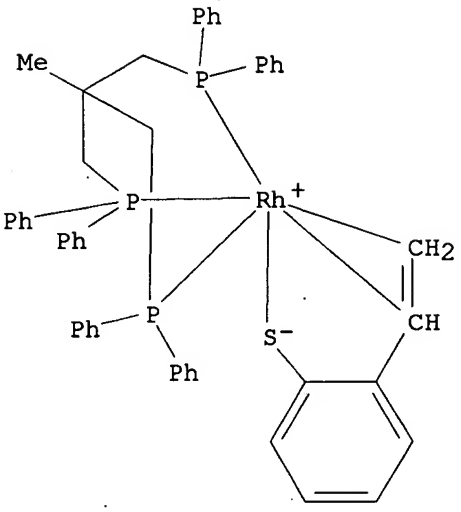


CM 2

CRN 16919-18-9
CMF F6 P
CCI CCS



IT 164222-20-2
RL: CAT (Catalyst use); CPS (Chemical process); PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent); USES (Uses)
(Hydrogenation of quinoline by rhodium catalysts modified with the tripodal polyphosphine ligand MeC(CH2PPh2)3)
RN 164222-20-2 CAPLUS
CN Rhodium, [[2-[(diphenylphosphino-κP)methyl]-2-methyl-1,3-propanediyl]bis[diphenylphosphine-κP]][2-(η2-ethenyl)benzenethiolato-κS]- (9CI) (CA INDEX NAME)



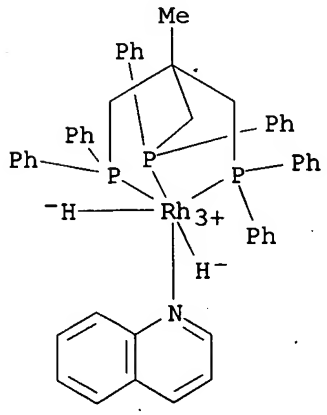

IT 405072-79-9P
RL: CAT (Catalyst use); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(Hydrogenation of quinoline by rhodium catalysts modified with the tripodal polyphosphine ligand MeC(CH2PPh2)3)

RN 405072-79-9 CAPLUS

CN Rhodium(1+), [[2-[(diphenylphosphino-κP)methyl]-2-methyl-1,3-propanediyl]bis[diphenylphosphine-κP]]dihydro(quinoline)-, (OC-6-33)-, hexafluorophosphate(1-) (9CI) (CA INDEX NAME)

CM 1

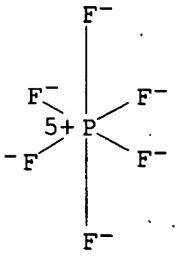
CRN 405072-78-8
CMF C50 H48 N P3 Rh
CCI CCS



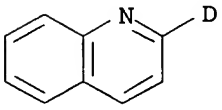

CM 2

CRN 16919-18-9

CMF F6 P
CCI CCS

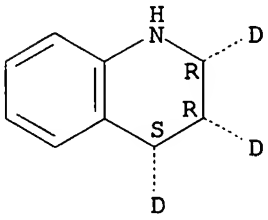


IT 15793-81-4P, Quinoline-2-d
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
(Hydrogenation of quinoline by rhodium catalysts modified with the tripodal polyphosphine ligand MeC(CH2PPh2)3)
RN 15793-81-4 CAPLUS
CN Quinoline-2-d (8CI, 9CI) (CA INDEX NAME)



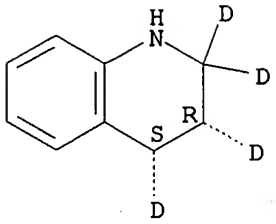
IT 405072-89-1P 405072-90-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(Hydrogenation of quinoline by rhodium catalysts modified with the tripodal polyphosphine ligand MeC(CH2PPh2)3)
RN 405072-89-1 CAPLUS
CN Quinoline-2,3,4-d3, 1,2,3,4-tetrahydro-, (2R,3R,4S)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 405072-90-4 CAPLUS
CN Quinoline-2,3,4-d3, 1,2,3,4-tetrahydro-2-d-, (3R,4S)-rel- (9CI) (CA INDEX NAME)

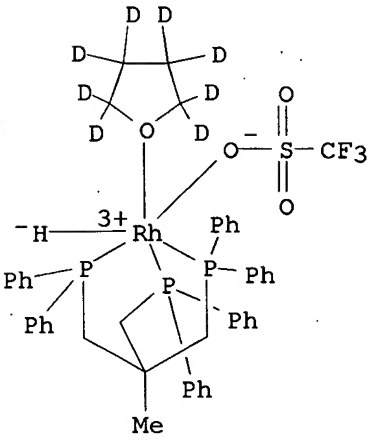
Relative stereochemistry.



IT 405072-83-5P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation) ; PREP (Preparation); RACT (Reactant or reagent)
(coordinative substitution; Hydrogenation of quinoline by rhodium catalysts modified with the tripodal polyphosphine ligand MeC(CH2PPh2)3)
RN 405072-83-5 CAPLUS
CN Rhodium(1+), [[2-[(diphenylphosphino-κP)methyl]-2-methyl-1,3-propanediyl]bis[diphenylphosphine-κP]]hydro(tetrahydro-d4-furan-d4)(trifluoromethanesulfonato-κO)-, (OC-6-43)-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

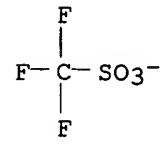
CM 1

CRN 405072-82-4
CMF C46 H40 D8 F3 O4 P3 Rh S
CCI CCS



CM 2

CRN 37181-39-8
CMF C F3 O3 S



REFERENCE COUNT: 118 THERE ARE 118 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 28 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2001:194193 CAPLUS
DOCUMENT NUMBER: 135:5779
TITLE: Aqueous micellar and non-micellar effects during the asymmetric hydrogenation of dehydroamino acid derivatives: influence of amphiphiles on enantioselectivity and α-CH/CD exchange
AUTHOR(S): Grassert, I.; Oehme, G.
CORPORATE SOURCE: Institut fur Organische Katalyseforschung an der Universitat Rostock e.V., Rostock, D-18055, Germany
SOURCE: Journal of Organometallic Chemistry (2001), 621(1-2), 158-165
CODEN: JORCAI; ISSN: 0022-328X
PUBLISHER: Elsevier Science S.A.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The effect of different amphiphiles on the CH/CD exchange in the homogeneously catalyzed asym. hydrogenation/deuteration of Me (Z)-α-acetamidocinnamate or Me α-acetamidoacrylate in an aqueous micellar medium has been investigated in connection with the effect of amphiphiles on the enhancement of enantioselectivity. In comparison with the exchange of α-CH/CD in water, the amphiphiles inhibit the reaction in the order: cationic<zwitterionic«anionic. In mixts. of cationic [cetyltrimethylammonium hydrogen sulfate, C16H33N(Me)3+HSO4-] and anionic amphiphiles (sodium dodecyl sulfate, SDS) the H/D-exchange amount is low in the presence of an excess of SDS, but it increases rapidly near a CTA+HSO4- mole fraction of 0.5 to give a high level of exchange. The enantioselectivity drops to a min. in the 1:1 mixture because of the low solubility of the cationic-anionic aggregates and the absence of micelles. The results obtained with mixed micelles of Brij 35 [polyethyleneoxide(23) monododecylether] and SDS are quite different. This mixture is dispersible and able to form micelles over the entire range of mole fractions (0 to 1). As a consequence, the isotope exchange is almost constant from a mole fraction of 0.3-0.9 of SDS. The enantioselectivity is nearly constant over the whole range. The inhibition of H/D exchange in the presence of long-chain alkyl sulfates seems to be caused by a specific interaction with the catalytic rhodium complex.

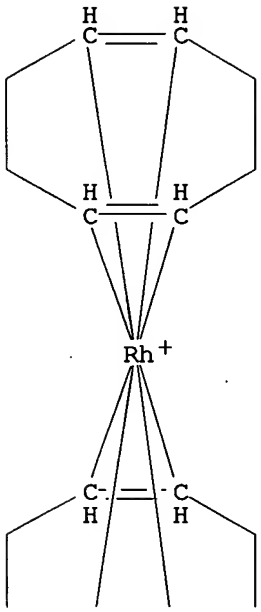
IT 35138-22-8
RL: CAT (Catalyst use); USES (Uses)
(effect of amphiphiles on the enantioselectivity and α-CH/CD exchange during the rhodium-catalyzed, asym. hydrogenation of dehydroamino acid derivs.)

RN 35138-22-8 CAPLUS
CN Rhodium(1+), bis[(1,2,5,6-η)-1,5-cyclooctadiene]-, tetrafluoroborate(1-) (1:1) (CA INDEX NAME)

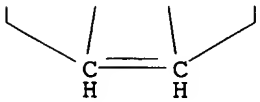
CM 1

CRN 35015-47-5
CMF C16 H24 Rh
CCI CCS

PAGE 1-A

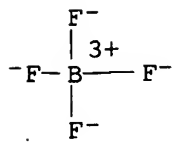


PAGE 2-A



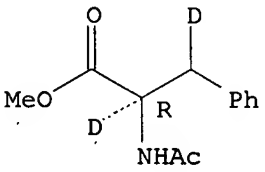
CM 2

CRN 14874-70-5
CMF B F4
CCI CCS



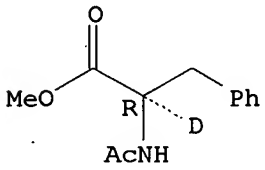
IT 342036-00-4P
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
(effect of amphiphiles on the enantioselectivity and α-CH/CD exchange during the rhodium-catalyzed, asym. hydrogenation of dehydroamino acid derivs.)
RN 342036-00-4 CAPLUS
CN D-Phenylalanine-α,β-d2, N-acetyl-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.




IT 290350-13-9P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(effect of amphiphiles on the enantioselectivity and α-CH/CD exchange during the rhodium-catalyzed, asym. hydrogenation of dehydroamino acid derivs.)
RN 290350-13-9 CAPLUS
CN D-Phenylalanine-α-d, N-acetyl-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.




REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 29 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2001:151108 CAPLUS
DOCUMENT NUMBER: 134:311325
TITLE: Hydrogen-deuterium exchange during the reductive deuteration of α- and γ-tocopherol chromenes
AUTHOR(S): Lei, Huangshu; Atkinson, Jeffrey
CORPORATE SOURCE: Institute for Molecular Catalysis, Department of Chemistry, Brock University, St. Catharines, ON, L2S 3A1, Can.
SOURCE: Journal of Labelled Compounds & Radiopharmaceuticals (2001), 44(3), 215-223
CODEN: JLCRD4; ISSN: 0362-4803
PUBLISHER: John Wiley & Sons Ltd.
DOCUMENT TYPE: Journal

LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:311325

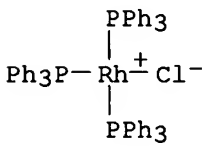
AB Reduction of tocopherol chromenes with heterogeneous catalysts and deuterium gas resulted in various degrees of deuterium incorporation despite the use of high purity deuterium gas. Exchange of hydrogens on C-7 of γ-tocopherol was evident by 2H-NMR and could be controlled by consideration of the substrate (chromene) to catalyst ratio, concentration and temperature Tocopherols deuterated at C3 and C4 were prepared with 94% d2 incorporation using 10% Pd/C at 0°C in Et acetate.

IT 7440-06-4, Platinum, uses 14694-95-2, Wilkinson's catalyst
RL: CAT (Catalyst use); USES (Uses)
(hydrogen-deuterium exchange during reductive deuteration of α- and γ-tocopherol chromenes)

RN 7440-06-4 CAPLUS
CN Platinum (CA INDEX NAME)

Pt

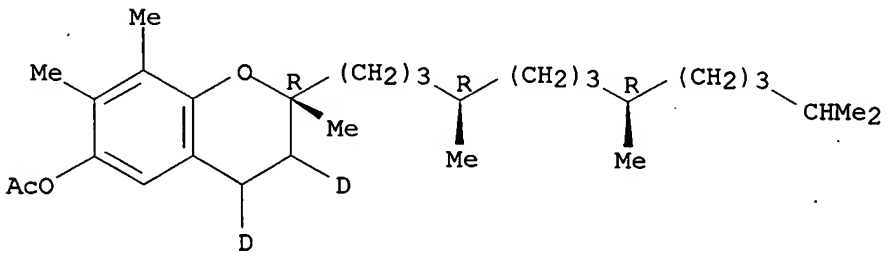
RN 14694-95-2 CAPLUS
CN Rhodium, chlorotris(triphenylphosphine)-, (SP-4-2)- (CA INDEX NAME)



IT 335203-18-4P 335203-19-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(hydrogen-deuterium exchange during reductive deuteration of α- and γ-tocopherol chromenes)

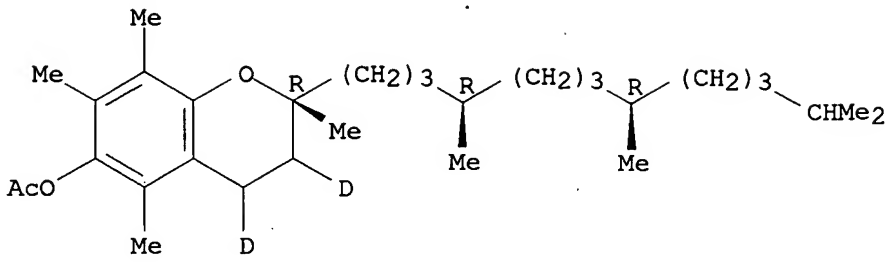
RN 335203-18-4 CAPLUS
CN 2H-1-Benzopyran-3,4-d2-6-ol, 3,4-dihydro-2,7,8-trimethyl-2-[(4R,8R)-4,8,12-trimethyltridecyl]-, acetate, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 335203-19-5 CAPLUS
CN 2H-1-Benzopyran-3,4-d2-6-ol, 3,4-dihydro-2,5,7,8-tetramethyl-2-[(4R,8R)-4,8,12-trimethyltridecyl]-, acetate, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



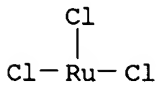
REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 30 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2001:112579 CAPLUS
DOCUMENT NUMBER: 134:366832
TITLE: A highly efficient synthetic procedure for deuterating imidazoles and imidazolium salts
AUTHOR(S): Hardacre, Christopher; McMath, S. E. Jane; Holbrey, John D.
CORPORATE SOURCE: School of Chemistry, The Queen's University of Belfast, Belfast, BT9 5AG, UK
SOURCE: Chemical Communications (Cambridge, United Kingdom) (2001), (4), 367-368
CODEN: CHCOFS; ISSN: 1359-7345
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:366832

AB Both substituted imidazoles and 1,3-dialkylimidazolium salts can be fully deuterated on the heterocyclic ring using D2O over heterogeneous Pd catalysts: deuterated 1-alkyl-3-methylimidazolium chloride and hexafluorophosphate ionic liqs. can also be prepared in good yields utilizing readily available and relatively low cost sources of deuterium. For example, alkylation of 1H-imidazole with methanol-d4 using ruthenium chloride hydrate/tributylphosphine as catalyst gave 1-(methyl-d3)-1H-imidazole (I). Palladium on activated carbon (2 g, 10% palladium) was reduced under dihydrogen for 1 h; then I ( (0.117 mmol) was dissolved in pure D2O (0.28 mmol) and added to the reduced catalyst. The mixture was degassed and heated to 100° for 1 h; the mixture was filtered and solvent was removed to give ring deuterated 1-(methyl-d3)-1H-imidazole-2,4,5-d3 (II) in 91% yield. Chloromethane-D3 (18.7 mmol) was condensed onto II in a tube and cooled to -180° with liquid nitrogen. Alkylation of I with iodoethane-d5 gave 1-(ethyl-d5)-3-(methyl-d3)-1H-imidazolium-2,4,5-d3 iodide. The tube was sealed, brought to room temperature and then heated to 80° for 15 h to give 1,3-di(methyl-d3)-1H-imidazolium-2,4,5-d3 chloride in 99% yield.

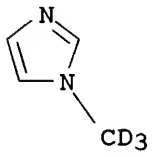
IT 10049-08-8, Ruthenium chloride (RuCl3)
RL: CAT (Catalyst use); USES (Uses)
(preparation of deuterated imidazole and imidazolium compds. (ionic liqs.) by palladium or platinum-catalyzed deuteration of imidazoles and imidazolium derivs.)

RN 10049-08-8 CAPLUS
CN Ruthenium chloride (RuCl3) (CA INDEX NAME)

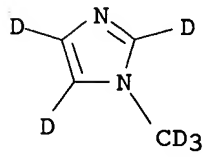


IT 7440-06-4P, Platinum, preparation
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation of deuterated imidazole and imidazolium compds. (ionic liqs.) by palladium or platinum-catalyzed deuteration of imidazoles and imidazolium derivs.)
RN 7440-06-4 CAPLUS
CN Platinum (CA INDEX NAME)

IT 16650-76-3P, 1-(Methyl-d3)-1H-imidazole
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of deuterated imidazole and imidazolium compds. (ionic liqs.) by palladium or platinum-catalyzed deuteration of imidazoles and imidazolium derivs.)
RN 16650-76-3 CAPLUS
CN 1H-Imidazole, 1-(methyl-d3)- (CA INDEX NAME)

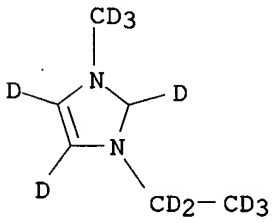


IT 285978-27-0P, 1-(Methyl-d3)-1H-imidazole-2,4,5-d3
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of deuterated imidazole and imidazolium compds. (ionic liqs.) by palladium or platinum-catalyzed deuteration of imidazoles and imidazolium derivs.)
RN 285978-27-0 CAPLUS
CN 1H-Imidazole-2,4,5-d3, 1-(methyl-d3)- (9CI) (CA INDEX NAME)



IT 340010-18-6P 340010-20-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of deuterated imidazole and imidazolium compds. (ionic liqs.) by palladium or platinum-catalyzed deuteration of imidazoles and imidazolium salts)
RN 340010-18-6 CAPLUS

CN 1H-Imidazolium-2,4,5-d3, 1-(ethyl-d5)-3-(methyl-d3)-, iodide (9CI) (CA INDEX NAME)



● $I^-$

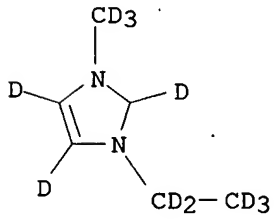
ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 340010-20-0 CAPLUS

CN 1H-Imidazolium-2,4,5-d3, 1-(ethyl-d5)-3-(methyl-d3)-, hexafluorophosphate(1-) (9CI) (CA INDEX NAME)

CM 1

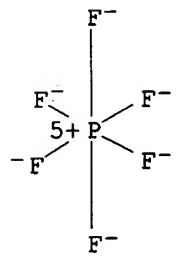
CRN 340010-19-7
CMF C6 D11 N2



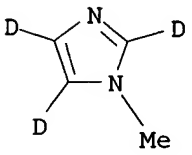
ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

CM 2

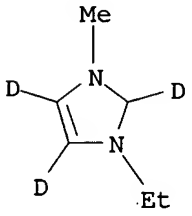
CRN 16919-18-9
CMF F6 P
CCI CCS



IT 4166-68-1P 160203-50-9P 160203-52-1P
340010-15-3P 340010-16-4P 340010-17-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of deuterated imidazole and imidazolium compds. (ionic liqs.) by palladium or platinum-catalyzed deuteration of imidazoles and imidazolium salts)
RN 4166-68-1 CAPLUS
CN 1H-Imidazole-2,4,5-d3, 1-methyl- (9CI) (CA INDEX NAME)

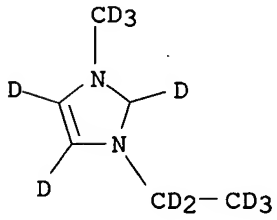



RN 160203-50-9 CAPLUS
CN 1H-Imidazolium-2,4,5-d3, 1-ethyl-3-methyl-, chloride (9CI) (CA INDEX NAME)




● $Cl^-$

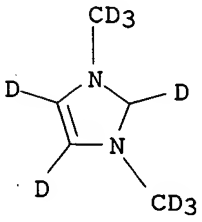
ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 160203-52-1 CAPLUS
CN 1H-Imidazolium-2,4,5-d3, 1-(ethyl-d5)-3-(methyl-d3)-, chloride (9CI) (CA INDEX NAME)




● $Cl^-$

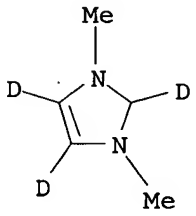
ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

RN 340010-15-3 CAPLUS
CN 1H-Imidazolium-2,4,5-d3, 1,3-di(methyl-d3)-, chloride (9CI) (CA INDEX NAME)



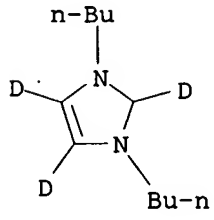
● $Cl^-$

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 340010-16-4 CAPLUS
CN 1H-Imidazolium-2,4,5-d3, 1,3-dimethyl-, chloride (9CI) (CA INDEX NAME)



● $Cl^-$

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE
RN 340010-17-5 CAPLUS
CN 1H-Imidazolium-2,4,5-d3, 1,3-dibutyl-, chloride (9CI) (CA INDEX NAME)



● $Cl^-$

ONE OR MORE TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

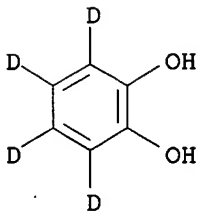
L24 ANSWER 31 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2000:549991 CAPLUS
DOCUMENT NUMBER: 134:147329
TITLE: Convenient synthesis of deuterated cycloalkanes from polyhalophenols with nickel-aluminum alloy in alkaline deuterium oxide
AUTHOR(S): Tsuzuki, Hirohisa; Mataka, Shuntaro; Tashiro, Masashi
CORPORATE SOURCE: Center of Advanced Instrumental Analysis, Kyusha University, Kasuga, 816, Japan
SOURCE: Synthesis and Applications of Isotopically Labelled Compounds 1997, Proceedings of the International Symposium, 6th, Philadelphia, PA, United States, Sept. 14-18, 1997 (1998), Meeting Date 1997, 203-206. Editor(s): Heys, J. Richard; Melillo, David G. John Wiley & Sons Ltd.: Chichester, UK.
CODEN: 69AGFQ
DOCUMENT TYPE: Conference
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:147329

AB A symposium report on the deuteration of polyhalophenolic substrates in the presence of nickel-aluminum alloy.

IT 11114-68-4
RL: CAT (Catalyst use); USES (Uses)
(deuterated cycloalkanes from polyhalophenols with nickel-aluminum alloy in alkaline deuterium oxide)
RN 11114-68-4 CAPLUS
CN Aluminum alloy, nonbase, Al,Ni (CA INDEX NAME)

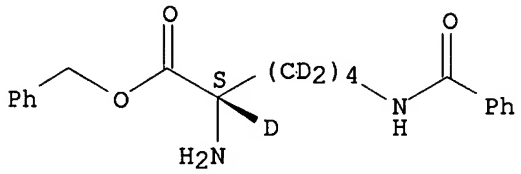
| Component | Component Registry Number |
|---|---|
| Al | 7429-90-5 |
| Ni | 7440-02-0 |

IT 103963-58-2P, 1,2-Benzene-3,4,5,6-d4-diol 324520-33-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(deuterated cycloalkanes from polyhalophenols with nickel-aluminum alloy in alkaline deuterium oxide)
RN 103963-58-2 CAPLUS
CN 1,2-Benzene-3,4,5,6-d4-diol (9CI) (CA INDEX NAME)



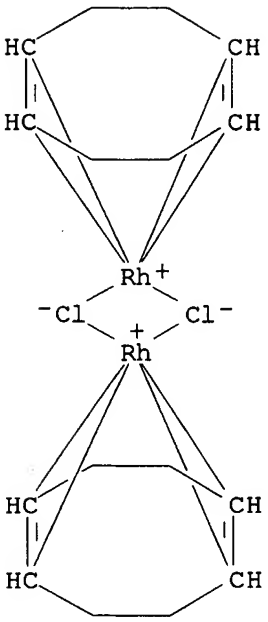

RN 324520-33-4 CAPLUS
CN L-Lysine-2,3,3,4,4,5,5,6,6-d9, N6-benzoyl-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



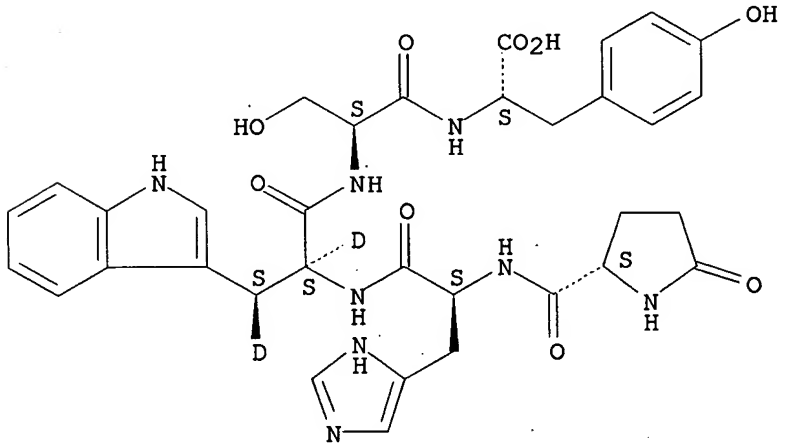
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 32 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2000:549990 CAPLUS
DOCUMENT NUMBER: 133:282061
TITLE: Peptide tritiation by homogeneous catalysis
AUTHOR(S): Hammadi, A.; Meunier, G.; Tarride, J. -L.; Menez, A.; Genet, R.
CORPORATE SOURCE: CEA, Department d'Ingenierie et d'Etudes des Proteines, Gif-sur-Yvette, F91191, Fr.
SOURCE: Synthesis and Applications of Isotopically Labelled Compounds 1997, Proceedings of the International Symposium, 6th, Philadelphia, PA, United States, Sept. 14-18, 1997 (1998), Meeting Date 1997, 197-201. Editor(s): Heys, J. Richard; Melillo, David G. John Wiley & Sons Ltd.: Chichester, UK.
CODEN: 69AGFQ
DOCUMENT TYPE: Conference
LANGUAGE: English
AB A symposium report. The stereoselective labeling by deuteration and tritiation of tryptophan-containing biol. peptides using chiral rhodium complexes as catalysts was discussed. Two examples of deuteration were given; biol. dehydropeptides, H-pGlu-His-ΔTrp-Ser-Tyr-OH (ΔTrp = cis-α,β-dehydro-tryptophan) and Boc-βAla-ΔTrp-Met-Asp-Phe-NH2, were prepared and asym. deuterated in the presence of chiral rhodium catalysts, generated in-situ from [Rh(COD)Cl]2 and chiral ligands (S,S)-Diop, (R,R)-Dpcb or (R,R)-Dipamp.
IT 12092-47-6, [Rh(COD)Cl]2
RL: CAT (Catalyst use); USES (Uses)
(asym. deuteration of dehydrotryptophanyl peptides by chiral rhodium catalysts)
RN 12092-47-6 CAPLUS
CN Rhodium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di- (CA INDEX NAME)



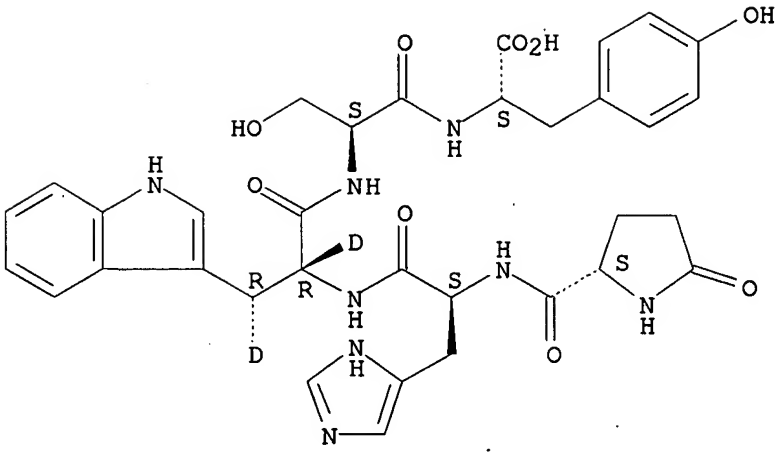
IT 207744-22-7P 207744-23-8P 207744-24-9P
207744-25-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(asym. deuteration of dehydrotryptophanyl peptides by chiral rhodium catalysts)
RN 207744-22-7 CAPLUS
CN L-Tyrosine, 5-oxo-L-prolyl-L-histidyl-L-tryptophyl-(βS)-α,β-d2-L-seryl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



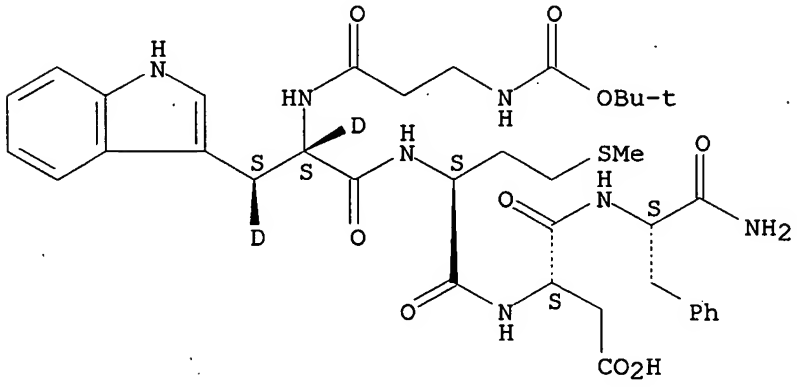
RN 207744-23-8 CAPLUS
CN L-Tyrosine, 5-oxo-L-prolyl-L-histidyl-D-tryptophyl-(βR)-α,β-d2-L-seryl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



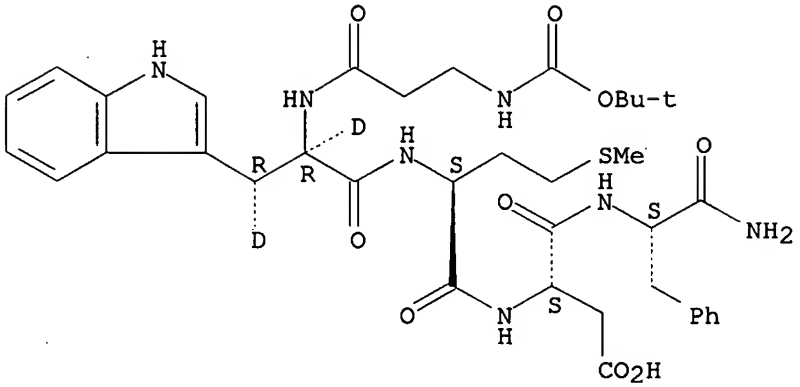
RN 207744-24-9 CAPLUS
CN 3-7-Cholecystokinin-7 (swine), 3-[N-[(1,1-dimethylethoxy)carbonyl]-β-alanine]-4-[L-tryptophan-(βS)-α,β-d2]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 207744-25-0 CAPLUS
CN 3-7-Cholecystokinin-7 (swine), 3-[N-[(1,1-dimethylethoxy)carbonyl]-β-alanine]-4-[D-tryptophan-(βR)-α,β-d2]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 33 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1999:512220 CAPLUS
DOCUMENT NUMBER: 131:286361
TITLE: Deuteration of indole and N-methylindole by Raney nickel catalysis
AUTHOR(S): Yau, Wai-Ming; Gawrisch, Klaus
CORPORATE SOURCE: LMBB, NIAAA, NIH, Rockville, MD, 20852, USA
SOURCE: Journal of Labelled Compounds & Radiopharmaceuticals (1999), 42(7), 709-713
CODEN: JLCRD4; ISSN: 0362-4803
PUBLISHER: John Wiley & Sons Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

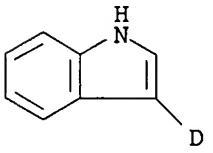
AB Indole and N-methylindole were partially or fully deuterated by Raney nickel catalyzed 1H2H exchange in a series of deuterated solvents. Perdeuterated indoles have been obtained in water and methanol while compds. that are preferentially deuterated at specific sites were obtained in chloroform, acetone, acetonitrile, ethanol, and isopropanol. The partially deuterated compds. are an important research tool for solid-state NMR studies on proteins.

IT 7440-02-0, Raney nickel, uses
RL: CAT (Catalyst use); USES (Uses)
(catalysts; deuteration of indole and N-methylindole by Raney nickel)
RN 7440-02-0 CAPLUS
CN Nickel (CA INDEX NAME)

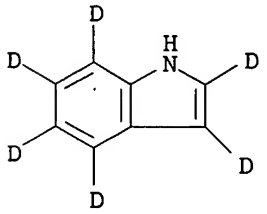
Ni

IT 57754-36-6P, 1H-Indole-3-d 104959-27-5P, 1H-Indole-2,3,4,5,6,7-d6 158953-96-9P, 1-Methyl-1H-Indole-3-d 210100-66-6P 246048-74-8P, 1H-Indole-2,3,7-d3 246048-77-1P, 1-Methyl-1H-Indole-2,3,4-d3 246048-79-3P, 1-Methyl-d3-1H-Indole-2,3,5,7-d4 246048-82-8P, 1-Methyl-d3-1H-Indole-2,3,4,5,6,7-d6
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

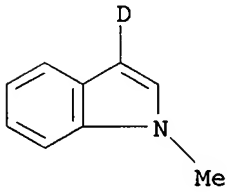
RN 57754-36-6 CAPLUS
CN 1H-Indole-3-d (9CI) (CA INDEX NAME)



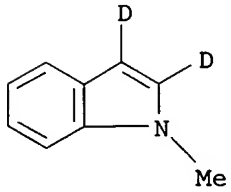
RN 104959-27-5 CAPLUS
CN 1H-Indole-2,3,4,5,6,7-d6 (CA INDEX NAME)



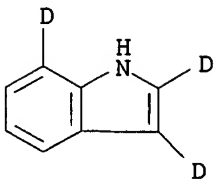
RN 158953-96-9 CAPLUS
CN 1H-Indole-3-d, 1-methyl- (CA INDEX NAME)



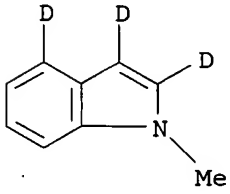
RN 210100-66-6 CAPLUS
CN 1H-Indole-2,3-d2, 1-methyl- (9CI) (CA INDEX NAME)



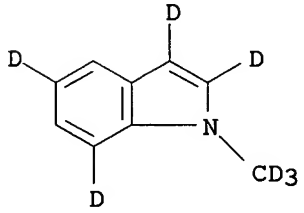
RN 246048-74-8 CAPLUS
CN 1H-Indole-2,3,7-d3 (9CI) (CA INDEX NAME)



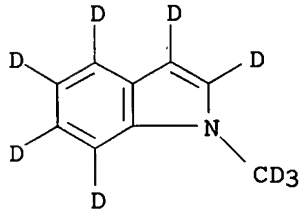
RN 246048-77-1 CAPLUS
CN 1H-Indole-2,3,4-d3, 1-methyl- (9CI) (CA INDEX NAME)



RN 246048-79-3 CAPLUS
CN 1H-Indole-2,3,5,7-d4, 1-(methyl-d3)- (9CI) (CA INDEX NAME)



RN 246048-82-8 CAPLUS
CN 1H-Indole-2,3,4,5,6,7-d6, 1-(methyl-d3)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 34 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1999:297574 CAPLUS
DOCUMENT NUMBER: 131:87507
TITLE: Rhodium-catalyzed hydroformylation of vinylidenic olefins: the different behaviors of the isomeric

alkyl-metal intermediates as the origin of the β-regioselectivity

AUTHOR(S): Lazzaroni, Raffaello; Settambolo, Roberta; Uccello-Barretta, Gloria; Caiazzo, Aldo; Scamuzzi, Simone

CORPORATE SOURCE: Dipartimento di Chimica e Chimica Industriale, Centro di Studio per le Macromolecole Stereordinate ed Otticamente Attive, Pisa, 56126, Italy

SOURCE: Journal of Molecular Catalysis A: Chemical (1999), 143(1-3), 123-130
CODEN: JMCCF2; ISSN: 1381-1169

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

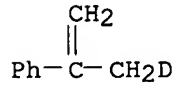
LANGUAGE: English

AB The β-regioselective hydroformylation of the vinylidenic olefins 2-phenylpropene (1a), 2-methylpropene (1b) and 2,3,3-trimethylbutene (1c) was investigated via deuterioformylation expts. [100°C, 100 atm, $Rh_4(CO)_{12}$] carried out at partial substrate conversion. The crude reaction mixts. were directly submitted to 2H NMR analyses. The results obtained allowed to conclude that whereas the primary rhodium-alkyl intermediate undergoes migratory insertion on CO, giving the corresponding linear aldehyde, the tertiary rhodium-alkyl intermediate, when it does form (i.e., in the case of 1a and 1b but not in the case of 1c), undergoes β-hydride elimination exclusively, accounting for the almost complete β-regioselectivity.

IT 64976-23-4P 69912-51-2P 97732-76-8P
230298-14-3P
RL: PNU (Preparation, unclassified); PREP (Preparation)
(preparation of)

RN 64976-23-4 CAPLUS

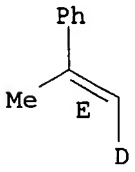
CN Benzene, [1-(methyl-d)ethenyl]- (9CI) (CA INDEX NAME)



RN 69912-51-2 CAPLUS

CN Benzene, [(1E)-1-methylethenyl-2-d]- (9CI) (CA INDEX NAME)

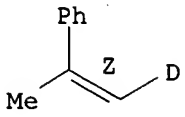
Double bond geometry as shown.



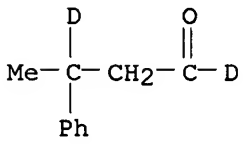
RN 97732-76-8 CAPLUS

CN Benzene, [(1Z)-1-methylethenyl-2-d]- (9CI) (CA INDEX NAME)

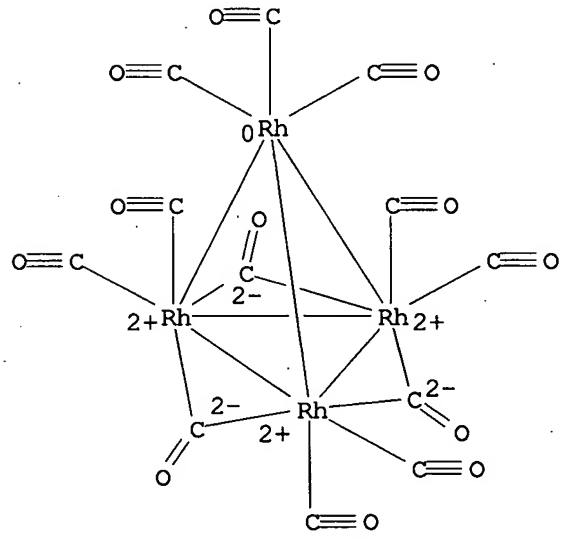
Double bond geometry as shown.



RN 230298-14-3 CAPLUS
CN Benzenepropanal-formyl,β-d2, β-methyl- (9CI) (CA INDEX NAME)



IT 19584-30-6, Tetrarhodium dodecacarbonyl
RL: CAT (Catalyst use); USES (Uses)
(rhodium-catalyzed hydroformylation of vinylidenic olefins)
RN 19584-30-6 CAPLUS
CN Rhodium, tri-μ-carbonylnonacarbonyltetra-, tetrahedro (CA INDEX NAME)



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 35 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1999:256017 CAPLUS
DOCUMENT NUMBER: 130:351827
TITLE: The NiCl2·2H2O-Li-arene combination as reducing system. 4. Dehalogenation of organic halides using the NiCl2·2H2O-Li-DTBB (cat.) combination
AUTHOR(S): Alonso, Francisco; Radivoy, Gabriel; Yus, Miguel
CORPORATE SOURCE: Departamento de Quimica Organica, Facultad de Ciencias, Universidad de Alicante, Alicante, E-03080,

Spain
SOURCE: Tetrahedron (1999), 55(14), 4441-4444
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 130:351827

AB The reaction of different chlorinated, brominated or iodinated materials, bearing or without a functional group, with a mixture of nickel(II) chloride dihydrate, an excess of lithium powder and a catalytic amount of 4,4'-di-tert-butylbiphenyl (DTBB) (5 mol%) in THF at room temperature, leads to the formation of the corresponding products resulting from a halogen/hydrogen exchange. The use of deuterium oxide instead of water in the nickel salt allows the corresponding deuteration. This methodol. does not work with fluorinated materials.

IT 17638-48-1, Nickel chloride (NiCl2) dihydrate 203518-65-4
, Nickel chloride (NiCl2) di(hydrate-d2)
RL: CAT (Catalyst use); USES (Uses)
(dehalogenation of aryl or alkyl halides using lithium/tert-butylbiphenyl and nickel chloride dihydrate)

RN 17638-48-1 CAPLUS
CN Nickel chloride (NiCl2), dihydrate (8CI, 9CI) (CA INDEX NAME)

Cl—Ni—Cl

●2 $H_2O$

RN 203518-65-4 CAPLUS
CN Nickel chloride (NiCl2), di(hydrate-d2) (9CI) (CA INDEX NAME)

Cl—Ni—Cl

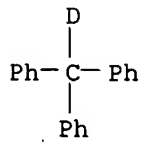
●2 $D_2O$

IT 1861-04-7P, (Ethyl-2-d)benzene 2913-53-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(dehalogenation of aryl or alkyl halides using lithium/tert-butylbiphenyl and nickel chloride dihydrate)

RN 1861-04-7 CAPLUS
CN Benzene, ethyl-2-d- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

$DCH_2—CH_2—Ph$

RN 2913-53-3 CAPLUS
CN Benzene, 1,1',1''-(methylidyne-d)tris- (9CI) (CA INDEX NAME)

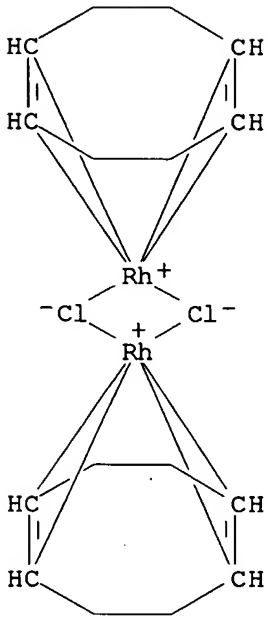


REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 36 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1997:752443 CAPLUS
DOCUMENT NUMBER: 128:13430
ORIGINAL REFERENCE NO.: 128:2621a,2624a
TITLE: Asymmetric deuteration of N-acetyl-(Z)-α,β-dehydrotryptophan-(L)-phenylalanine methyl ester produced by (L)-tryptophan 2',3'-oxidase from Chromobacterium violaceum. A new route for stereospecific labeling of peptides
AUTHOR(S): Hammadi, Akli; Menez, Andre; Genet, Roger
CORPORATE SOURCE: CEA/Saclay, Departement d'Ingenierie et d'Etudes des Proteines, Gif-sur-Yvette, F91191, Fr.
SOURCE: Tetrahedron (1997), 53(47), 16115-16122
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 128:13430

AB A novel approach to the synthesis of deuterium- and tritium-labeled peptides through the catalytic asym. reduction of (Z)-α,β-dehydrotryptophan (ΔzTrp)-containing peptides, using rhodium complexes with chiral diphosphine ligands as the catalysts, is described. Ac-ΔzTrp-L-Phe-OMe is used as a model substrate to study this new route. The dehydropeptide is produced by L-tryptophan 2',3'-oxidase from Chromobacterium violaceum in a single step reaction. Diastereomeric excesses up to 98 % have been obtained with (R,R)-dipamp as ligand in the catalyst. Extremely high stereoselectivities for producing the L,L- or D,L-isomer could be achieved using the appropriate chiral ligands. This method has good potential for stereospecific deuteration or tritiation of peptides.

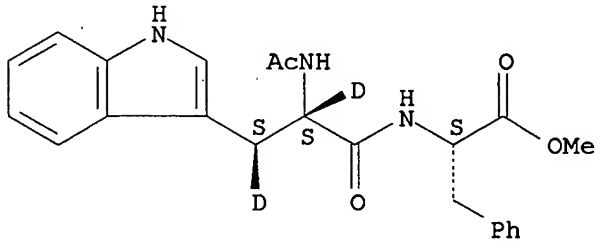
IT 12092-47-6, Cyclooctadienerhodium chloride dimer
RL: CAT (Catalyst use); USES (Uses)
(enzymic preparation and asym. deuteration of dehydrotryptophan-containing peptides)
RN 12092-47-6 CAPLUS
CN Rhodium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di- (CA INDEX NAME)




IT 199111-09-6P 199111-10-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(enzymic preparation and asym. deuteration of dehydrotryptophan-containing peptides)

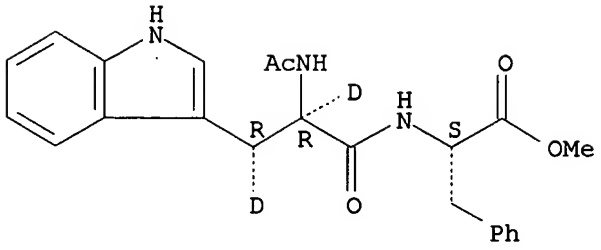
RN 199111-09-6 CAPLUS
CN L-Phenylalanine, N-acetyl-L-tryptophyl-(βS)-α,β-d2-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.




RN 199111-10-9 CAPLUS
CN L-Phenylalanine, N-acetyl-D-tryptophyl-(βR)-α,β-d2-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

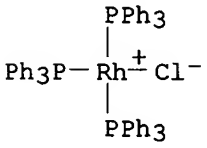



REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

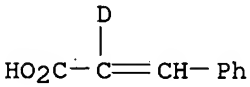
L24 ANSWER 37 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1997:324308 CAPLUS
DOCUMENT NUMBER: 127:17291
ORIGINAL REFERENCE NO.: 127:3489a,3492a
TITLE: First Evidence That the Mechanism of Catalytic Hydrogenation with Homogeneous Palladium and Rhodium Catalysts Is Strongly Influenced by Substrate Polarity
AUTHOR(S): Yu, Jinquan; Spencer, Jonathan B.
CORPORATE SOURCE: University Chemical Laboratory, University of Cambridge, Cambridge, CB2 1EW, UK
SOURCE: Journal of the American Chemical Society (1997), 119(22), 5257-5258
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB We have observed that when cis-alkenes are hydrogenated with homogeneous palladium and rhodium catalysts they readily isomerize to the trans-configuration with the incorporation of a deuterium atom. By studying how electron withdrawing and donating groups conjugated to the double bond influence the location of deuterium addition we have been able to gain a clear insight into how the metal hydrogen bond in the catalyst is polarized just prior to adding to the cis-alkene. Remarkably, the result demonstrate that the palladium hydrogen bond is capable of being polarized in either mode (a Pdδ+-Hδ- or b Pdδ--Hδ+) depending on the coulombic properties of the substrate, whereas the rhodium catalyst studied is dominated by mode a (Rhδ+-Hδ-). This provides strong evidence that the mechanism of catalytic hydrogenation is a 2 electron process that can be dramatically affected by the substrate's polarity.

IT 14694-95-2, Chlorotris(triphenylphosphine)rhodium
RL: CAT (Catalyst use); PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent); USES (Uses)
(strong substrate polarity effect on mechanism of catalytic hydrogenation with homogeneous palladium and rhodium catalysts)
RN 14694-95-2 CAPLUS
CN Rhodium, chlorotris(triphenylphosphine)-, (SP-4-2)- (CA INDEX NAME)

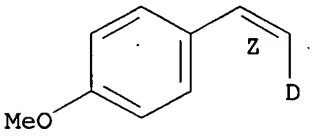


IT 69104-43-4P 89039-12-3P 89039-13-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(strong substrate polarity effect on mechanism of catalytic hydrogenation with homogeneous palladium and rhodium catalysts)
RN 69104-43-4 CAPLUS
CN 2-Propenoic-2-d acid, 3-phenyl- (9CI) (CA INDEX NAME)



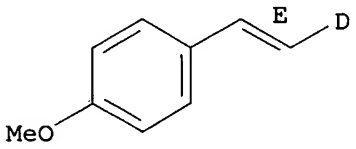
RN 89039-12-3 CAPLUS
CN Benzene, 1-[(1Z)-ethenyl-2-d]-4-methoxy- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 89039-13-4 CAPLUS
CN Benzene, 1-[(1E)-ethenyl-2-d]-4-methoxy- (CA INDEX NAME)

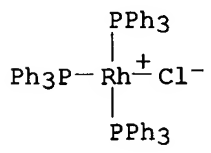
Double bond geometry as shown.



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

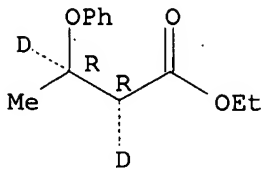
L24 ANSWER 38 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1997:164817 CAPLUS
DOCUMENT NUMBER: 126:143805
ORIGINAL REFERENCE NO.: 126:27793a,27796a
TITLE: Diastereoselectivity of Enolate Anion Protonation. H/D Exchange of β-Substituted Ethyl Butanoates in Ethanol-d
AUTHOR(S): Mohrig, Jerry R.; Rosenberg, Robert E.; Apostol, John W.; Bastienaansen, Mark; Evans, Jordan W.; Franklin, Sonya J.; Frisbie, C. Daniel; Hirose, Christopher B.;

Hunstad, David A.; James, Thomas L.; King, Randall W.; Larson, Christopher J.; Fu, Sabrina S.; Owen, David A.; Hamm, Michelle L.; Warnet, Ronald; Latham, Hallie A.; Stein, Karin A.
CORPORATE SOURCE: Department of Chemistry, Carleton College, Northfield, MN, 55057, USA
SOURCE: Journal of the American Chemical Society (1997), 119(3), 479-486
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 126:143805
AB The stereochem. of base-catalyzed H/D exchange on 13 β-substituted Et butanoates in ethanol-d has been studied in order to analyze the steric and electronic factors which control the diastereoselectivity of electrophilic attack on enolate anions. Electrophilic deuteration of the enolate anion also dets. the stereoselectivity of 1,4-conjugate addition of ethanol-d to α,β-unsatd. esters. Exptl. conditions were selected which rigorously exclude the effects of ion pairing and aggregation. The research showed that stereoelectronic factors generally produce higher stereoselection than steric effects do. Electroneg. heteroatom substituents at C-3 produced a 10:1 ratio of the 2R*,3R*/2R*,3S* 2-deuteriobutanoates. In the most stable transition states for electrophilic attack, these electroneg. substituents occupy an antiperiplanar position to the forming C-D bond. Only with a β-tert-Bu substituent did steric effects produce high stereoselection, and it fell off rapidly with a decrease in carbon branching. Protonation of acyclic β-ethoxy aldehyde and ketone enolates follows the same diastereoselectivity pattern as the β-ethoxy ester enolate, but protonation of the cyanocarbanion from a β-ethoxy nitrile gives much lower stereoselection.
IT 14694-95-2, Tris(triphenylphosphine)rhodium(I) chloride
RL: CAT (Catalyst use); USES (Uses)
(H/D exchange of β-substituted Et butanoates in ethanol-d and diastereoselectivity of enolate anion protonation)
RN 14694-95-2 CAPLUS
CN Rhodium, chlorotris(triphenylphosphine)-, (SP-4-2)- (CA INDEX NAME)



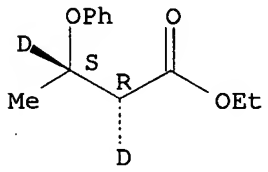
IT 186517-49-7P 186517-50-0P 186517-59-9P
186517-60-2P
RL: PNU (Preparation, unclassified); PRP (Properties); PREP (Preparation)
(H/D exchange of β-substituted Et butanoates in ethanol-d and diastereoselectivity of enolate anion protonation)
RN 186517-49-7 CAPLUS
CN Butanoic-2,3-d2 acid, 3-phenoxy-, ethyl ester, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



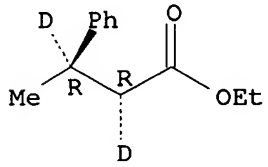
RN 186517-50-0 CAPLUS
CN Butanoic-2,3-d2 acid, 3-phenoxy-, ethyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



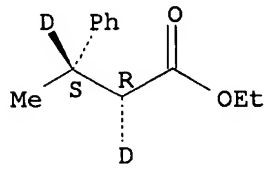
RN 186517-59-9 CAPLUS
CN Benzenepropanoic-α,β-d2 acid, β-methyl-, ethyl ester, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 186517-60-2 CAPLUS
CN Benzenepropanoic-α,β-d2 acid, β-methyl-, ethyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 63 THERE ARE 63 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 39 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1996:688097 CAPLUS
DOCUMENT NUMBER: 126:103765
ORIGINAL REFERENCE NO.: 126:20017a

TITLE: Rhodium- and palladium-catalyzed proton exchange in styrene detected in situ by para-hydrogen induced polarization

AUTHOR(S): Harthun, Andreas; Giernoth, Ralf; Elsevier, Cornelis J.; Bargon, Joachim

CORPORATE SOURCE: Inst. Phys. Theor. Chem., Univ. Bonn, Bonn, D-53115, Germany

SOURCE: Chemical Communications (Cambridge) (1996), (21), 2483-2484
CODEN: CHCOFS; ISSN: 1359-7345

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

AB In situ NMR spectroscopy of para-hydrogen induced nuclear polarization shows a pairwise proton exchange mechanism in styrene during homogeneous hydrogenation with rhodium(I) and palladium(0) catalysts.

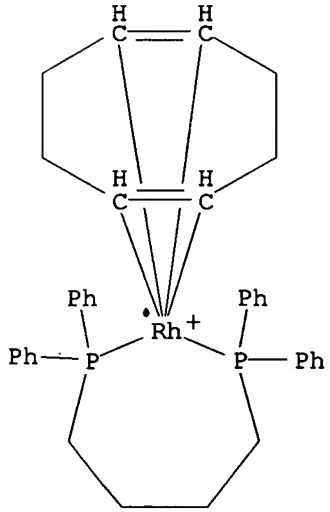
IT 79255-71-3
RL: CAT (Catalyst use); PEP (Physical, engineering or chemical process); PROC (Process); USES (Uses)
(rhodium- and palladium-catalyzed proton exchange in styrene detected in situ by para-hydrogen induced polarization)

RN 79255-71-3 CAPLUS

CN Rhodium(1+), [1,1'-(1,4-butanediyl)bis[1,1-diphenylphosphine-κP]][(1,2,5,6-η)-1,5-cyclooctadiene]-, tetrafluoroborate(1-) (1:1) (CA INDEX NAME)

CM 1

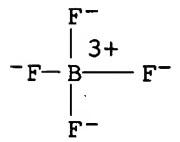
CRN 75752-92-0
CMF C36 H40 P2 Rh
CCI CCS



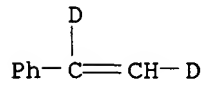

CM 2

CRN 14874-70-5
CMF B F4

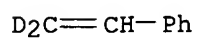
CCI CCS



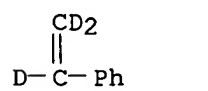
IT 60052-92-8P, Styrene-α,β-d2
RL: PEP (Physical, engineering or chemical process); PNU (Preparation, unclassified); PRP (Properties); RCT (Reactant); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
(rhodium- and palladium-catalyzed proton exchange in styrene detected in situ by para-hydrogen induced polarization)
RN 60052-92-8 CAPLUS
CN Benzene, ethenyl-1,2-d2- (9CI) (CA INDEX NAME)



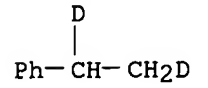
IT 934-85-0P, Styrene-β,β-d2 3814-93-5P, Styrene-α,β,β-d3 119721-67-4P
RL: PNU (Preparation, unclassified); PRP (Properties); PREP (Preparation)
(rhodium- and palladium-catalyzed proton exchange in styrene detected in situ by para-hydrogen induced polarization)
RN 934-85-0 CAPLUS
CN Benzene, ethenyl-2,2-d2- (CA INDEX NAME)



RN 3814-93-5 CAPLUS
CN Benzene, ethenyl-1,2,2-d3- (CA INDEX NAME)



RN 119721-67-4 CAPLUS
CN Benzene, ethyl-1,2-d2- (6CI, 9CI) (CA INDEX NAME)



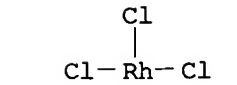
L24 ANSWER 40 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1996:338213 CAPLUS
DOCUMENT NUMBER: 125:10164
ORIGINAL REFERENCE NO.: 125:2249a,2252a
TITLE: Isotopic enrichment by asymmetric deuteration. An investigation of the synthesis of deuterated (S)-(-)-methylsuccinic acids from itaconic acid.
AUTHOR(S): Hardick, David J.; Blagbrough, Ian S.; Potter, Barry V. L.
CORPORATE SOURCE: School of Pharmacy and Pharmacology, University of Bath, Bath, BA2 7AY, UK
SOURCE: Journal of the American Chemical Society (1996), 118(25), 5897-5903
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

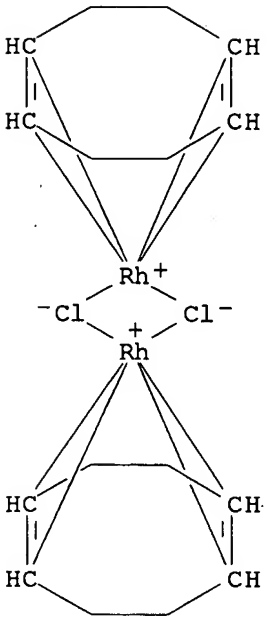
AB Two different asym. deuteration methodologies based on gaseous deuterium at 1 atm pressure and transfer deuteration from the decomposition of DCO2D in the presence of a Rh catalyst, have been used to prepare deuterium-enriched (S)-(-)-methylsuccinic acid. Complex labeling occurs as the result of an equilibrium which exists between the olefin and a catalyst-alkyl intermediate in a Wilkinson-type mechanism in which H or D may be bound to Rh. Enantiomeric excess was >90% and approx. 2.4 deuterons were incorporated; a ratio of 1.8:1 methyl:methine deuteration was observed, and there was no evidence for olefin isomerization into conjugation with both CO2H groups. These results have general applicability to the synthesis of isotopically labeled homochiral substituted carboxylic acids and also in interpreting the 13C NMR data which are generated by the simultaneous presence of several deuterium containing isotopomers.

IT 10049-07-7, Rhodium trichloride 12092-47-6, Rhodium 1,5-cyclooctadiene chloride dimer
RL: CAT (Catalyst use); USES (Uses)
(investigation of the synthesis of deuterated (S)-(-)-methylsuccinic acids from itaconic acid)

RN 10049-07-7 CAPLUS
CN Rhodium chloride (RhCl3) (CA INDEX NAME)

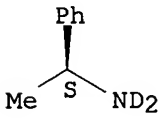


RN 12092-47-6 CAPLUS
CN Rhodium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di- (CA INDEX NAME)



IT 172821-56-6P
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(investigation of the synthesis of deuterated (S)-(-)-methylsuccinic acids from itaconic acid)
RN 172821-56-6 CAPLUS
CN Benzenemethanamine-d2, α-methyl-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 41 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1996:98985 CAPLUS
DOCUMENT NUMBER: 124:260517
ORIGINAL REFERENCE NO.: 124:48263a,48266a
TITLE: Retention of optical purity in H-D exchange reactions catalyzed by cobalt-aluminum alloy in Na2CO3-D2O
AUTHOR(S): Mukumoto, Mamoru; Tsuzuki, Hirohisa; Mataka, Shuntaro; Tashiro, Masashi; Tsukinoki, Takehito; Nagano, Yoshiaki
CORPORATE SOURCE: Dep. Mol. Sci. Technol., Kyushu Univ., Kasuga, 816, Japan
SOURCE: Chemistry Letters (1996), (2), 165-6
CODEN: CMLTAG; ISSN: 0366-7022
PUBLISHER: Nippon Kagakkai
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 124:260517

AB Co-Al alloy in a sodium carbonate-deuterium oxide solution catalyzes the H-D exchange reaction of optically active benzylic hydrogen atom without racemization. Thus, (R)-mandelic acid give Me α-D-(R)-mandelate in 89% yield with 99% enantiomeric excess.

IT 11114-55-9
RL: CAT (Catalyst use); USES (Uses)
(deuteration of benzylic compds. with retention of configuration using Co-Al alloy in Na2CO3-D2O)

RN 11114-55-9 CAPLUS

CN Aluminum alloy, nonbase, Al,Co (CA INDEX NAME)

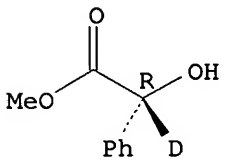
| Component | Component Registry Number |
|---|---|
| Al | 7429-90-5 |
| Co | 7440-48-4 |

IT 175289-31-3P 175289-32-4P 175289-33-5P
175289-34-6P 175289-35-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(deuteration of benzylic compds. with retention of configuration using Co-Al alloy in Na2CO3-D2O)

RN 175289-31-3 CAPLUS

CN Benzeneacetic-d acid, α-hydroxy-, methyl ester, (αR)- (9CI) (CA INDEX NAME)

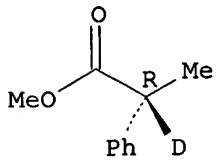
Absolute stereochemistry.




RN 175289-32-4 CAPLUS

CN Benzeneacetic-d acid, α-methyl-, methyl ester, (R)- (9CI) (CA INDEX NAME)

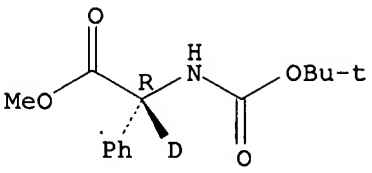
Absolute stereochemistry.




RN 175289-33-5 CAPLUS

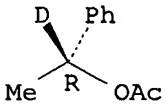
CN Benzeneacetic-d acid, α-[[(1,1-dimethylethoxy)carbonyl]amino]-, methyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



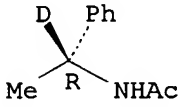
RN 175289-34-6 CAPLUS
CN Benzenemethan-d-ol, α-methyl-, acetate, (αR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 175289-35-7 CAPLUS
CN Acetamide, N-[(1R)-1-phenylethyl-1-d]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

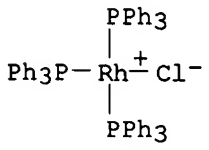


L24 ANSWER 42 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1995:633707 CAPLUS
DOCUMENT NUMBER: 123:144526
ORIGINAL REFERENCE NO.: 123:25773a,25776a
TITLE: Regio- and stereoselective deuteration of α,β-positions of amino acids
AUTHOR(S): Oba, Makoto; Nishiyama, Kozaburo
CORPORATE SOURCE: Dep. Mater. Sci. Technol., Tokai Univ., Numazu, Japan
SOURCE: Journal of Deuterium Science (1993), 3(2), 77-81
CODEN: JDSCFJ; ISSN: 0919-651X
PUBLISHER: Society of Deuterium Science
DOCUMENT TYPE: Journal
LANGUAGE: Japanese

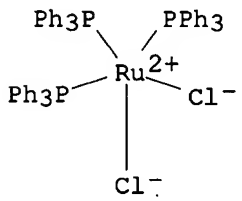
AB The regio- and stereoselective deuteration of α,β-positions of amino acids, which contribute to the determination of χ1-angle of side chains of peptide, was reported. The deuteration of dehydroamino acids, prepared by the Erlenmeyer method, was promoted by a transition metal catalyst such as Pd-C, RhCl(PPh3)3, and RuCl2(PPh3)3 in deuterated solvent (MeOD, AcOD etc). In these catalysts, Wilkinson type complex was more effective for regio- and stereoselective deuteration of dehydroamino acid, especially, leucine derivs. Furthermore, enantioselective deuteration using an optically active phosphine complex catalyst is now in progress.

IT 14694-95-2, Tris(triphenylphosphine)rhodium chloride
15529-49-4, Tris(triphenylphosphine)ruthenium dichloride

RL: CAT (Catalyst use); USES (Uses)
(regio- and stereoselective deuteration of α,β-positions of amino acids)
RN 14694-95-2 CAPLUS
CN Rhodium, chlorotris(triphenylphosphine)-, (SP-4-2)- (CA INDEX NAME)

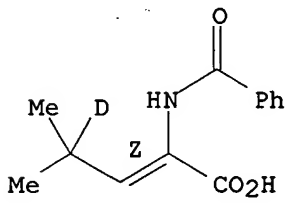


RN 15529-49-4 CAPLUS
CN Ruthenium, dichlorotris(triphenylphosphine)- (CA INDEX NAME)

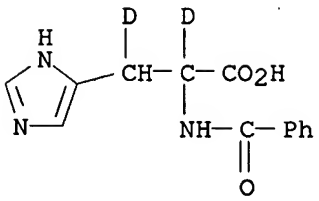


IT 165813-92-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(regio- and stereoselective deuteration of α,β-positions of amino acids)
RN 165813-92-3 CAPLUS
CN 2-Pentenoic-4-d acid, 2-(benzoylamino)-4-methyl-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

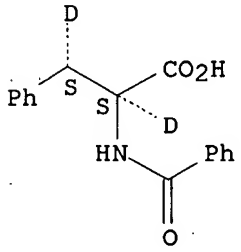


IT 57573-36-1P 68964-04-5P 165813-93-4P
165813-94-5P 165813-95-6P 165813-96-7P
166020-93-5P 170211-65-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(regio- and stereoselective deuteration of α,β-positions of amino acids)
RN 57573-36-1 CAPLUS
CN Histidine-α,β-d2, N-benzoyl-, (R*,S*)- (9CI) (CA INDEX NAME)



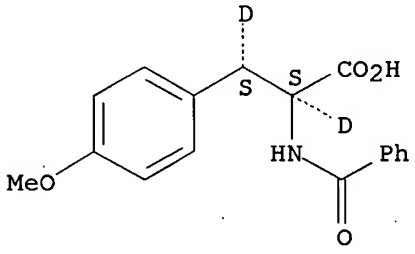
RN 68964-04-5 CAPLUS
CN Phenylalanine-α,β-d2, N-benzoyl-, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



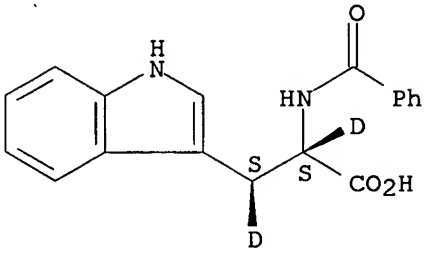
RN 165813-93-4 CAPLUS
CN Tyrosine-α,β-d2, N-benzoyl-O-methyl-, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



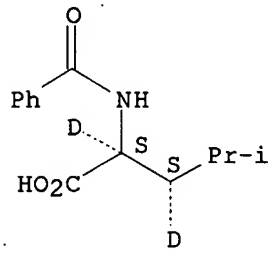
RN 165813-94-5 CAPLUS
CN Tryptophan-α,β-d2, N-benzoyl-, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



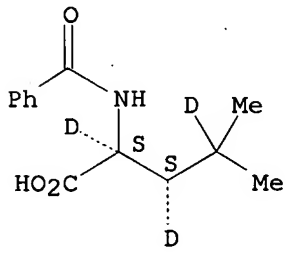
RN 165813-95-6 CAPLUS
CN Leucine-2,3-d2, N-benzoyl-, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



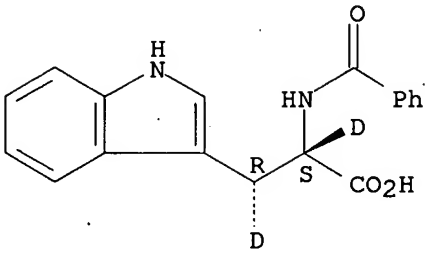
RN 165813-96-7 CAPLUS
CN Leucine-2,3,4-d3, N-benzoyl-, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

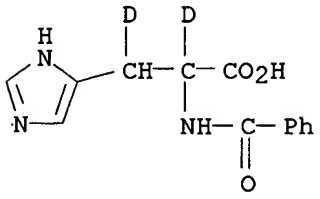


RN 166020-93-5 CAPLUS
CN Tryptophan-α,β-d2, N-benzoyl-, (R*,S*)- (9CI) (CA INDEX NAME)

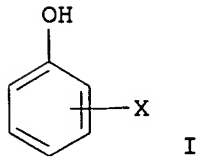
Relative stereochemistry.



RN 170211-65-1 CAPLUS
CN Histidine-α,β-d2, N-benzoyl-, (R*,R*)- (9CI) (CA INDEX NAME)



L24 ANSWER 43 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1995:630896 CAPLUS
DOCUMENT NUMBER: 123:285376
ORIGINAL REFERENCE NO.: 123:51139a,51142a
TITLE: Syntheses of phenol derivatives labeled with deuterium
AUTHOR(S): Tsuzuki, Hirohisa; Tashiro, Masashi
CORPORATE SOURCE: Cent. Adv. Instrumental Anal., Kyushu Univ., Kasuga, Japan
SOURCE: Journal of Deuterium Science (1993), 3(1), 28-32
CODEN: JDSCFJ; ISSN: 0919-651X
PUBLISHER: Society of Deuterium Science
DOCUMENT TYPE: Journal
LANGUAGE: Japanese
GI



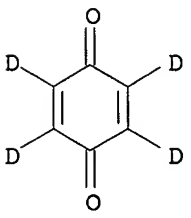
I

AB Reduction of halogenated phenol derivs. with Raney alloy/NaOD-D2O gave the corresponding deuterium-labeled catechols and hydroquinones with high isotope purity. Thus, halophenols I (X = 4-Br, 2,3,4,5,6-Cl5) were treated with Ni-Al alloy in 10% NaOD-D2O to give I (X = 4-D, 2,3,4,5,6-D5). Reaction of I (X = 2,3,4,5,6-D5) with Ni-Al alloy in 0.55

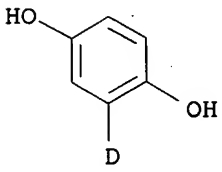
N BaO-D2O under ultrasound irradiation gave [2H11]cyclohexanol.
IT 12635-27-7
RL: CAT (Catalyst use); USES (Uses)
(syntheses of phenol derivs. labeled with deuterium)
RN 12635-27-7 CAPLUS
CN Aluminum alloy, base, Al 50,Ni 50 (CA INDEX NAME)

| Component | Component Percent | Component Registry Number |
|---|---|---|
| Al | 50 | 7429-90-5 |
| Ni | 50 | 7440-02-0 |

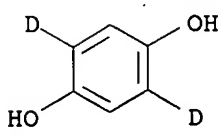
IT 2237-14-1P, 2,5-Cyclohexadiene-1,4-dione-2,3,5,6-d4
25285-27-2P, 1,4-Benzene-2-d-diol 25285-28-3P,
1,4-Benzene-2,5-d2-diol 25285-29-4P, 1,4-Benzene-2,3,5-d3-diol
25294-85-3P, 1,4-Benzene-2,3,5,6-d4-diol
RL: RCT (Reactant); SPN (Synthetic preparation); PREP
(Preparation); RACT (Reactant or reagent)
(syntheses of phenol derivs. labeled with deuterium)
RN 2237-14-1 CAPLUS
CN 2,5-Cyclohexadiene-1,4-dione-2,3,5,6-d4 (9CI) (CA INDEX NAME)



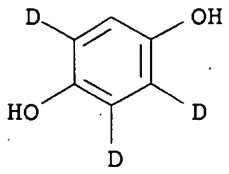

RN 25285-27-2 CAPLUS
CN 1,4-Benzene-2-d-diol (9CI) (CA INDEX NAME)



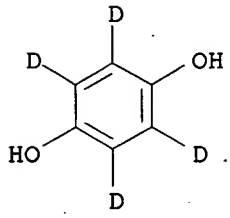

RN 25285-28-3 CAPLUS
CN 1,4-Benzene-2,5-d2-diol (9CI) (CA INDEX NAME)



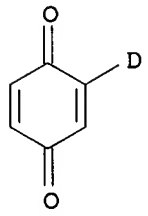

RN 25285-29-4 CAPLUS
CN 1,4-Benzene-2,3,5-d3-diol (9CI) (CA INDEX NAME)



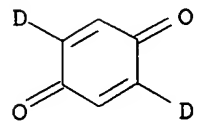
RN 25294-85-3 CAPLUS
CN 1,4-Benzene-2,3,5,6-d4-diol (9CI) (CA INDEX NAME)



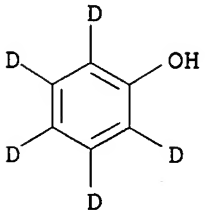
IT 2237-15-2P, 2,5-Cyclohexadiene-1,4-dione-2-d 2237-16-3P, 2,5-Cyclohexadiene-1,4-dione-2,5-d2 4165-62-2P, Phen-d5-ol 23951-03-3P, Phen-4-d-ol 51994-68-4P, 2,5-Cyclohexadiene-1,4-dione-2,3,5-d3 103963-58-2P, 1,2-Benzene-3,4,5,6-d4-diol
RL: SPN (Synthetic preparation); PREP (Preparation)
(syntheses of phenol derivs. labeled with deuterium)
RN 2237-15-2 CAPLUS
CN 2,5-Cyclohexadiene-1,4-dione-2-d (CA INDEX NAME)



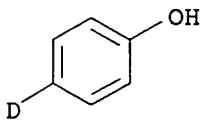
RN 2237-16-3 CAPLUS
CN 2,5-Cyclohexadiene-1,4-dione-2,5-d2 (9CI) (CA INDEX NAME)



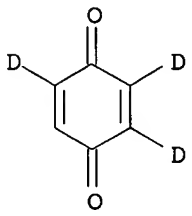
RN 4165-62-2 CAPLUS
CN Phen-2,3,4,5,6-d5-ol (CA INDEX NAME)



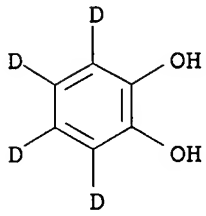
RN 23951-03-3 CAPLUS
CN Phen-4-d-ol (CA INDEX NAME)



RN 51994-68-4 CAPLUS
CN 2,5-Cyclohexadiene-1,4-dione-2,3,5-d3 (9CI) (CA INDEX NAME)



RN 103963-58-2 CAPLUS
CN 1,2-Benzene-3,4,5,6-d4-diol (9CI) (CA INDEX NAME)



L24 ANSWER 44 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1995:346830 CAPLUS
DOCUMENT NUMBER: 122:105421
ORIGINAL REFERENCE NO.: 122:19831a,19834a
TITLE: Method for producing deuterated aromatic compounds
INVENTOR(S): Kakinami, Takaaki; Eguchi, Hisao
PATENT ASSIGNEE(S): Tosoh Corp, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.

CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| JP 06228014 | A | 19940816 | JP 1993-12356 | 19930128 |

PRIORITY APPLN. INFO.: JP 1993-12356 19930128
OTHER SOURCE(S): CASREACT 122:105421

AB A halogenated aromatic compound is treated with a Raney alloy in D2O in the presence of alkali metal carbonate and/or alkaline earth metal carbonate to give a deuterated aromatic compound, which is useful as a pharmaceutical, an agrochem., a functional material, and a tracer for anal. This deuteration process is economical and of general application. Thus, 30 mL 10% Na2CO3-D2O solution was added to 0.87 g 2-bromophenol (I) followed by adding portion wise 1.0 g Raney Cu-Al alloy over .apprx.30 min at 40° and the resulting mixture was ripened at 60° for 1 h, filtered for removal of insol. materials such as the catalyst, acidified to pH .apprx.1 by adding concentrated HCl, and extracted with CH2Cl2 to give, after drying over MgSO4 and evaporation, 0.41 g colorless liquid containing unreacted I 4, 2-deuteriophenol 90, and dideuterated I 6%. Also prepared was 2,4-dideuteriobenzoic acid by reaction of 2-bromo-4-chlorobenzoic acid with D2O in the presence of Raney Ni and Na2CO3.

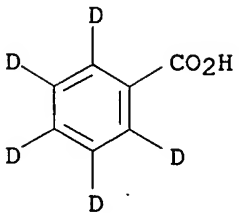
IT 7440-02-0, Raney nickel, uses
RL: CAT (Catalyst use); USES (Uses)
(preparation of deuterated aromatic compds. by deuteration of halogenated aromatic compds. in heavy water in presence of Raney nickel or copper)

RN 7440-02-0 CAPLUS
CN Nickel (CA INDEX NAME)

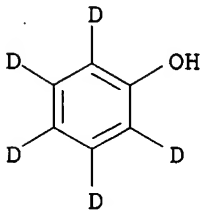
Ni

IT 1079-02-3P, Pentadeuteriobenzoic acid 4165-62-2P, Pentadeuteriophenol 23951-01-1P, 2-Deuteriophenol 57193-23-4P, Benzoic-2,4-d2 acid 160825-02-5P, Phen-2,?-d2-ol 160825-03-6P, Phen-2,?,?-d3-ol 160825-04-7P, Benzoic-2,4,?-d3 acid 160825-05-8P, Benzoic-2,4,?,?-d4 acid 160825-06-9P, Phen-2,?,?,?-d4-ol
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of deuterated aromatic compds. by deuteration of halogenated aromatic compds. in heavy water in presence of Raney nickel or copper)

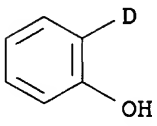
RN 1079-02-3 CAPLUS
CN Benzoic-2,3,4,5,6-d5 acid (CA INDEX NAME)



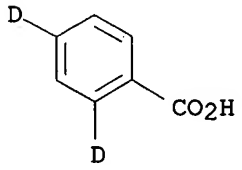
RN 4165-62-2 CAPLUS
CN Phen-2,3,4,5,6-d5-ol (CA INDEX NAME)



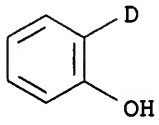
RN 23951-01-1 CAPLUS
CN Phen-2-d-ol (9CI) (CA INDEX NAME)



RN 57193-23-4 CAPLUS
CN Benzoic-2,4-d2 acid (9CI) (CA INDEX NAME)

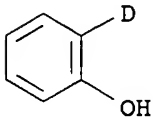


RN 160825-02-5 CAPLUS
CN Phen-2,?-d2-ol (9CI) (CA INDEX NAME)

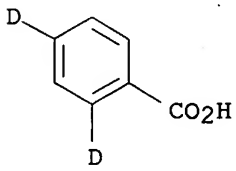


RN 160825-03-6 CAPLUS

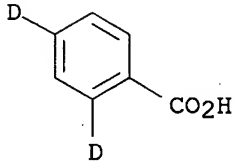
CN Phen-2,?,?-d3-ol (9CI) (CA INDEX NAME)



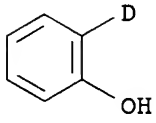
RN 160825-04-7 CAPLUS
CN Benzoic-2,4,?-d3 acid (9CI) (CA INDEX NAME)



RN 160825-05-8 CAPLUS
CN Benzoic-2,4,?,?-d4 acid (9CI) (CA INDEX NAME)

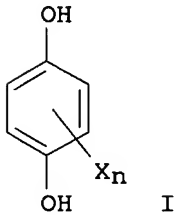


RN 160825-06-9 CAPLUS
CN Phen-2,?,?,?-d4-ol (9CI) (CA INDEX NAME)



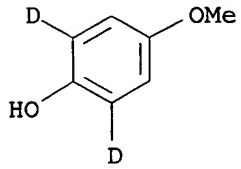
L24 ANSWER 45 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1995:45260 CAPLUS
DOCUMENT NUMBER: 122:55680
ORIGINAL REFERENCE NO.: 122:10787a,10790a
TITLE: Reductive dehalogenation and ring saturation of halogenated hydroquinones, pyrocatechol and resorcinol with Raney alloys in NaOD-D2O solution leading to hydroquinones, cyclohexane-1,4-diol and cyclohexane-1,3-dione labeled with deuterium
AUTHOR(S): Tsuzuki, Hirohisa; Iyama, Hironobu; Tsukinoki, Takehito; Mukumoto, Mamoru; Yonemitsu, Tadashi; Nagano, Yoshiaki; Thiemann, Thies; Mataka, Shuntaro; Tashiro, Masashi
CORPORATE SOURCE: Center of Advanced Instrumental Analysis, Kyushu

University, Kasuga, 816, Japan
SOURCE: Journal of Chemical Research, Synopses (1994), (8), 302-3
CODEN: JRPSDC; ISSN: 0308-2342
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 122:55680
GI

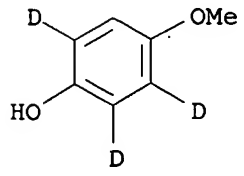


I

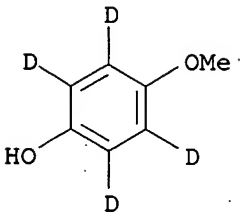
AB A versatile approach to the title compds. with Raney alloy/NaOD-D2O as the reducing system at 60-70 was described and the mechanism of catalysis discussed. Thus, bromohydroquinones (I; Xn =2-Br,2,5-Br2,2,3,5-Br3,2,3,5,6-Cl4) were treated with CuAl alloy in 10% NaOD-D2O at 60-70° for 1 h to give the corresponding I (Xn=2-D1, 2,5-D2,2,3,5-D3,2,3,5,6-D4) with > 84% isotopic purity.
IT 25474-90-2P 159839-22-2P 159839-23-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(reductive dehalogenation of halogenated methoxyphenol with Raney alloys in NaOD-D2O)
RN 25474-90-2 CAPLUS
CN Phen-2,6-d2-ol, 4-methoxy- (8CI, 9CI) (CA INDEX NAME)



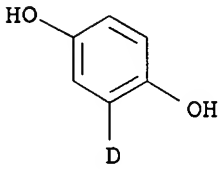

RN 159839-22-2 CAPLUS
CN Phen-2,3,6-d3-ol, 4-methoxy- (9CI) (CA INDEX NAME)



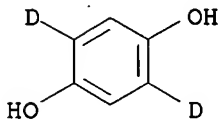

RN 159839-23-3 CAPLUS
CN Phen-2,3,5,6-d4-ol, 4-methoxy- (9CI) (CA INDEX NAME)



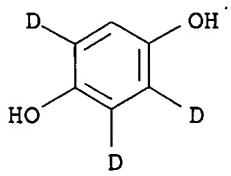
IT 25285-27-2P, 1,4-Benzene-2-d-diol 25285-28-3P, 1,4-Benzene-2,5-d2-diol 25285-29-4P, 1,4-Benzene-2,3,5-d3-diol 25294-85-3P, 1,4-Benzene-2,3,5,6-d4-diol
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(reductive dehalogenation of hydroquinones with Raney alloys in NaOD-D2O)
RN 25285-27-2 CAPLUS
CN 1,4-Benzene-2-d-diol (9CI) (CA INDEX NAME)



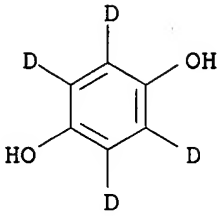
RN 25285-28-3 CAPLUS
CN 1,4-Benzene-2,5-d2-diol (9CI) (CA INDEX NAME)



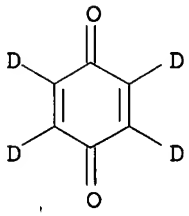
RN 25285-29-4 CAPLUS
CN 1,4-Benzene-2,3,5-d3-diol (9CI) (CA INDEX NAME)



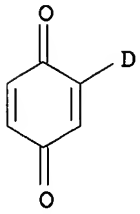
RN 25294-85-3 CAPLUS
CN 1,4-Benzene-2,3,5,6-d4-diol (9CI) (CA INDEX NAME)



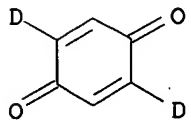
IT 2237-14-1P, 2,5-Cyclohexadiene-1,4-dione-2,3,5,6-d4
2237-15-2P, 2,5-Cyclohexadiene-1,4-dione-2-d 2237-16-3P,
2,5-Cyclohexadiene-1,4-dione-2,5-d2 2237-17-4P,
2,5-Cyclohexadiene-1,4-dione-2,6-d2 51994-68-4P,
2,5-Cyclohexadiene-1,4-dione-2,3,5-d3
RL: SPN (Synthetic preparation); PREP (Preparation)
(reductive dehalogenation of hydroquinones with Raney alloys in NaOD-D2O)
RN 2237-14-1 CAPLUS
CN 2,5-Cyclohexadiene-1,4-dione-2,3,5,6-d4 (9CI) (CA INDEX NAME)



RN 2237-15-2 CAPLUS
CN 2,5-Cyclohexadiene-1,4-dione-2-d (CA INDEX NAME)

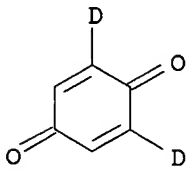


RN 2237-16-3 CAPLUS
CN 2,5-Cyclohexadiene-1,4-dione-2,5-d2 (9CI) (CA INDEX NAME)

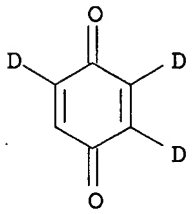


RN 2237-17-4 CAPLUS

CN 2,5-Cyclohexadiene-1,4-dione-2,6-d2 (9CI) (CA INDEX NAME)



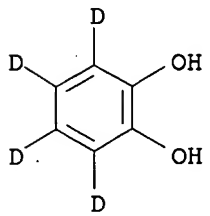
RN 51994-68-4 CAPLUS
CN 2,5-Cyclohexadiene-1,4-dione-2,3,5-d3 (9CI) (CA INDEX NAME)



IT 12635-27-7
RL: CAT (Catalyst use); USES (Uses)
(ring saturation of halogenated hydroquinones with Raney alloys in NaOD-D2O)
RN 12635-27-7 CAPLUS
CN Aluminum alloy, base, Al 50,Ni 50 (CA INDEX NAME)

| Component | Component Percent | Component Registry Number |
|---|---|---|
| Al | 50 | 7429-90-5 |
| Ni | 50 | 7440-02-0 |

IT 103963-58-2P, 1,2-Benzene-3,4,5,6-d4-diol
RL: SPN (Synthetic preparation); PREP (Preparation)
(ring saturation of halogenated hydroquinones with Raney alloys in NaOD-D2O)
RN 103963-58-2 CAPLUS
CN 1,2-Benzene-3,4,5,6-d4-diol (9CI) (CA INDEX NAME)



L24 ANSWER 46 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1992:173517 CAPLUS
DOCUMENT NUMBER: 116:173517

ORIGINAL REFERENCE NO.: 116:29355a,29358a
TITLE: On deuterium-labeling studies for probing rhodium-catalyzed hydroboration reactions [Erratum to document cited in CA114(21):206508c]
AUTHOR(S): Burgess, Kevin; Van der Donk, Wilfred A.; Kook, Alan M.
CORPORATE SOURCE: Rice Univ., Houston, TX, 77251, USA
SOURCE: Journal of Organic Chemistry (1991), 56(26), 7360
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Addnl. discussions of the deuterioborations reported in the original article have been provided. The error was not reflected in the abstract or the index entries.
IT 12092-46-5 68932-69-4
RL: CAT (Catalyst use); USES (Uses)
(catalyst, for deuteroboration of alkenes, regiochem. of (Erratum))
RN 12092-46-5 CAPLUS
CN Rhodium, dichlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]- (CA INDEX NAME)

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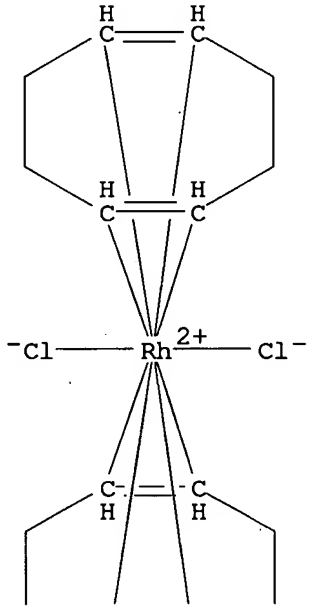


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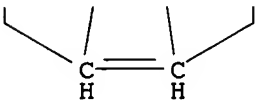
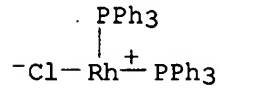
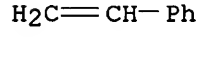



RN 68932-69-4 CAPLUS

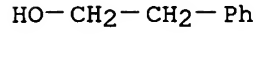
CN Rhodium, chlorobis(triphenylphosphine)- (CA INDEX NAME)



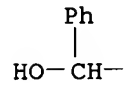
IT 45574-34-3P, preparation
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in rhodium-catalyzed deuteroboration of styrene (Erratum))
RN 45574-34-3 CAPLUS
CN Benzene, ethenyl-, labeled with deuterium (CA INDEX NAME)



IT 133496-75-0P 133496-76-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by rhodium-catalyzed deuteroboration of styrene (Erratum))
RN 133496-75-0 CAPLUS
CN Benzeneethanol, labeled with deuterium (9CI) (CA INDEX NAME)



RN 133496-76-1 CAPLUS
CN Benzenemethanol, α-methyl-, labeled with deuterium (CA INDEX NAME)



L24 ANSWER 47 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1991:206508 CAPLUS
DOCUMENT NUMBER: 114:206508
ORIGINAL REFERENCE NO.: 114:34815a,34818a
TITLE: On deuterium-labeling studies for probing rhodium-catalyzed hydroboration reactions
AUTHOR(S): Burgess, Kevin; Van der Donk, Wilfred A.; Kook, Alan M.
CORPORATE SOURCE: Rice Univ., Houston, TX, 77251, USA
SOURCE: Journal of Organic Chemistry (1991), 56(9), 2949-51
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Reactions of deuterocatecholborane (I) with alkenes in the presence of rhodium(+1) complexes have been reinvestigated. Distributions of label in the products differ significantly from those reported previously, and alternative rationales for these observations are provided. Thus, CH2:CMeCHMeOSiMe2CMe3 was treated with I in THF in the presence of RhCl(PPh3)3 to give, after oxidative workup, HOCH2CDMeCHMeOSiMe2CMe3 as

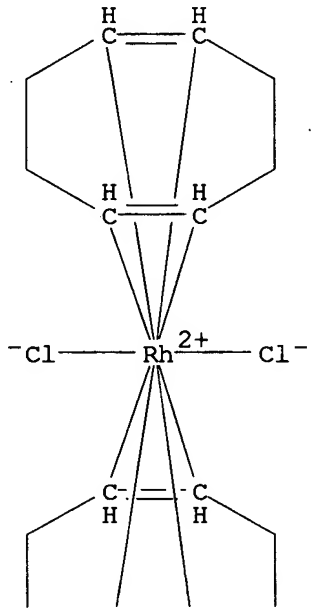
98% of the deuterated product.

IT 12092-46-5 68932-69-4, Bis(triphenylphosphine)rhodium chloride
RL: CAT (Catalyst use); USES (Uses)
(catalyst, for deuteroboration of alkenes, regiochem. of)

RN 12092-46-5 CAPLUS

CN Rhodium, dichlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]- (CA INDEX NAME)

PAGE 1-A



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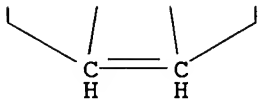
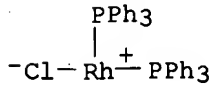


RN 68932-69-4 CAPLUS

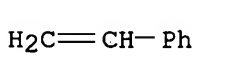
CN Rhodium, chlorobis(triphenylphosphine)- (CA INDEX NAME)



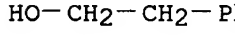
IT 45574-34-3P, preparation
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in rhodium-catalyzed deuteroboration of styrene)

RN 45574-34-3 CAPLUS

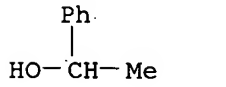
CN Benzene, ethenyl-, labeled with deuterium (CA INDEX NAME)



IT 133496-75-0P 133496-76-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by rhodium-catalyzed deuteroboration of styrene)
RN 133496-75-0 CAPLUS
CN Benzeneethanol, labeled with deuterium (9CI) (CA INDEX NAME)



RN 133496-76-1 CAPLUS
CN Benzenemethanol, α-methyl-, labeled with deuterium (CA INDEX NAME)



L24 ANSWER 48 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1991:142291 CAPLUS
DOCUMENT NUMBER: 114:142291
ORIGINAL REFERENCE NO.: 114:24129a,24132a
TITLE: Preparation of deuterated organic compounds
INVENTOR(S): Moebius, Guenter; Schaaf, Guenther
PATENT ASSIGNEE(S): Akademie der Wissenschaften der DDR, Ger. Dem. Rep.
SOURCE: Ger. (East), 3 pp.
CODEN: GEXXA8
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| DD 279376 | A3 | 19900606 | DD 1984-259704 | 19840130 |

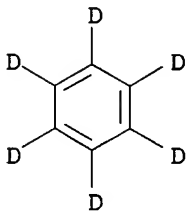
PRIORITY APPLN. INFO.: DD 1984-259704 19840130

AB C6-8 aliphatic hydrocarbons as well as Decalin and dioxane are deuterated to >99 atom% D by exposure to D2 and D2O at 423-563 K and 2-25 MPa in the presence of an appropriate gas-phase catalyst. Thus, 1 mol pure n-hexane was autoclaved with 10 mol D2O and 35 g 15% Pt-C catalyst under 10 MPa D2 at 488 K for 60 h. Both D2 and D2O were removed and replaced, and the process repeated 7 addnl. times, to give n-hexane with ≥99 atom-% D. Using 15% Pd-C catalyst, Decalin and dioxane were similarly deuterated.

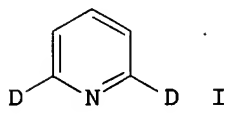
IT 7440-06-4, Platinum, uses and miscellaneous
RL: CAT (Catalyst use); USES (Uses)
(catalyst, for deuteration of aliphatic hydrocarbons, Decalin, and dioxane)
RN 7440-06-4 CAPLUS
CN Platinum (CA INDEX NAME)

Pt

IT 1076-43-3P, Benzene-d6
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 1076-43-3 CAPLUS
CN Benzene-1,2,3,4,5,6-d6 (CA INDEX NAME)



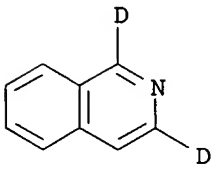
L24 ANSWER 49 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1990:631172 CAPLUS
DOCUMENT NUMBER: 113:231172
ORIGINAL REFERENCE NO.: 113:39001a,39004a
TITLE: Deuteration of pyridine derivatives: a very mild procedure
AUTHOR(S): Rubottom, George M.; Evain, Eric J.
CORPORATE SOURCE: Dep. Chem., Univ. Idaho, Moscow, ID, 83843, USA
SOURCE: Tetrahedron (1990), 46(15), 5055-64
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



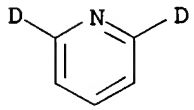
AB Ruthenium on carbon selectively catalyzes the hydrogen-deuterium exchange of pyridine derivs. at the ortho position. The reaction takes place at ambient temperature under mild conditions. Thus, pyridine in D3COD was stirred under 22 psi of D2 in the presence of 5% Ru-C to give ≥ 90% 2,6-dideuteropyridine (I).
IT 7440-18-8, Ruthenium, uses and miscellaneous
RL: CAT (Catalyst use); USES (Uses)
(catalyst, for regioselective hydrogen-deuterium exchange reaction of pyridines and isoquinoline)
RN 7440-18-8 CAPLUS
CN Ruthenium (CA INDEX NAME)

Ru

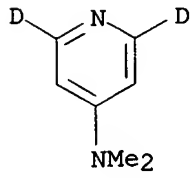
IT 130720-97-7P, 1,3-Dideuterioisoquinoline
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by ruthenium-catalyzed hydrogen-deuterium exchange reaction of isoquinoline)
RN 130720-97-7 CAPLUS
CN Isoquinoline-1,3-d2 (9CI) (CA INDEX NAME)



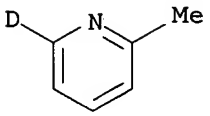
IT 17265-96-2P, 2,6-Dideuteropyridine 22527-01-1P, 2,6-Dideuterio-4-(dimethylamino)pyridine 79272-00-7P, 6-Deuterio-2-methylpyridine 130720-95-5P, 2,6-Dideuterio-3-methylpyridine 130720-96-6P, 6-Deuterio-2-ethylpyridine 130720-98-8P, 6-Deuterio-2-fluoropyridine
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by ruthenium-catalyzed hydrogen-deuterium exchange reaction of pyridine)
RN 17265-96-2 CAPLUS
CN Pyridine-2,6-d2 (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



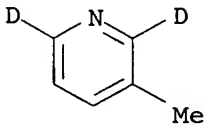
RN 22527-01-1 CAPLUS
CN 4-Pyridin-2,6-d2-amine, N,N-dimethyl- (9CI) (CA INDEX NAME)



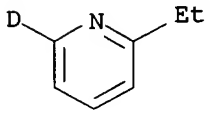
RN 79272-00-7 CAPLUS
CN Pyridine-2-d, 6-methyl- (9CI) (CA INDEX NAME)



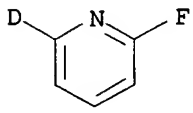
RN 130720-95-5 CAPLUS
CN Pyridine-2,6-d2, 3-methyl- (9CI) (CA INDEX NAME)



RN 130720-96-6 CAPLUS
CN Pyridine-2-d, 6-ethyl- (9CI) (CA INDEX NAME)



RN 130720-98-8 CAPLUS
CN Pyridine-2-d, 6-fluoro- (9CI) (CA INDEX NAME)

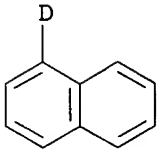


L24 ANSWER 50 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1990:531636 CAPLUS
DOCUMENT NUMBER: 113:131636
ORIGINAL REFERENCE NO.: 113:22351a,22354a
TITLE: Preparation of deuterated naphthalenes, anilines, m-toluidines, and anisoles by reductive dehalogenation of the corresponding halogenated derivatives with Raney copper-aluminum alloy in an alkaline deuterium oxide solution
AUTHOR(S): Tashiro, Masashi; Tsuzuki, Hirohisa; Tsukinoki, Takehito; Mataka, Shuntaro; Nakayama, Kouji; Yonemitsu, Tadashi
CORPORATE SOURCE: Inst. Adv. Mater. Study, Kyushu Univ., Kasuga, 816, Japan
SOURCE: Journal of Labelled Compounds and Radiopharmaceuticals (1990), 28(6), 703-12
CODEN: JLCRD4; ISSN: 0362-4803
DOCUMENT TYPE: Journal
LANGUAGE: English

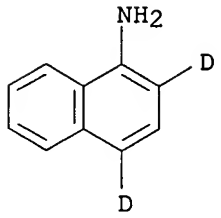
OTHER SOURCE(S): CASREACT 113:131636
AB Four deuterated naphthalenes, 10 deuterated anilines, 3 deuterated m-toluidine derivs., and 5 deuterated anisoles were prepared in high isotopic purities from the corresponding bromo or chloro precursors by reductive dehalogenation with Raney Cu-Al alloy in D2O containing NaOD. E.g., 2-BrC6H4NH2 gave 75% 2-DC6H4NH2 in 97% isotopic purity.
IT 11101-28-3
RL: CAT (Catalyst use); USES (Uses)
(Raney catalyst, for deuteration of bromonaphthalenes, bromo- and chloroaniline derivs., and bromoanisole derivs.)
RN 11101-28-3 CAPLUS
CN Copper alloy, nonbase, Cu,Ni (CA INDEX NAME)

| Component | Component Registry Number |
|---|---|
| Cu | 7440-50-8 |
| Ni | 7440-02-0 |

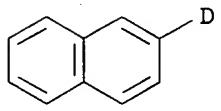
IT 875-62-7P, 1-Deuterionaphthalene 1683-99-4P, 1-Amino-2,4-dideuterionaphthalene 2430-34-4P, 2-Deuterionaphthalene 2567-25-1P, 2,4,6-Trideuterioanisole 7291-08-9P, 2,4,6-Trideuterioaniline 13122-28-6P, 4-Deuterioaniline 19617-82-4P, 3,5-Dideuterioaniline 19617-83-5P, 2,3,5,6-Tetradeuterioaniline 20938-43-6P, 4-Deuterioanisole 23878-49-1P, 1,5-Dideuterionaphthalene 26351-62-2P, 2-Deuterioanisole 50535-17-6P, 2-Deuterioaniline 50535-18-7P, 3-Deuterioaniline 68408-23-1P 120364-25-2P, 2,3-Dideuterioaniline 122258-85-9P, 2,4-Dideuterioaniline 129453-25-4P, 2,5-Dideuterioaniline 129453-26-5P, 2,6-Dideuterioaniline 129453-27-6P 129453-28-7P 129453-29-8P, 2,4-Dideuterioanisole 129453-30-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 875-62-7 CAPLUS
CN Naphthalene-1-d (CA INDEX NAME)



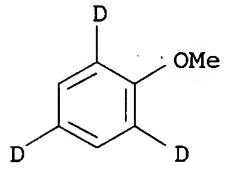

RN 1683-99-4 CAPLUS
CN 1-Naphthalen-2,4-d2-amine (9CI) (CA INDEX NAME)



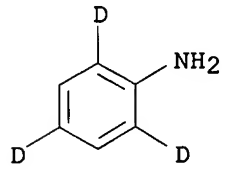
RN 2430-34-4 CAPLUS
CN Naphthalene-2-d (CA INDEX NAME)



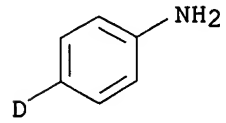
RN 2567-25-1 CAPLUS
CN Benzene-1,3,5-d3, 2-methoxy- (9CI) (CA INDEX NAME)



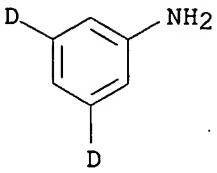
RN 7291-08-9 CAPLUS
CN Benzen-2,4,6-d3-amine (9CI) (CA INDEX NAME)



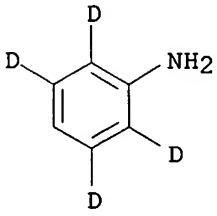
RN 13122-28-6 CAPLUS
CN Benzen-4-d-amine (9CI) (CA INDEX NAME)



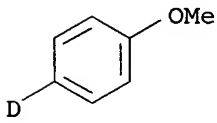
RN 19617-82-4 CAPLUS
CN Benzen-3,5-d2-amine (9CI) (CA INDEX NAME)



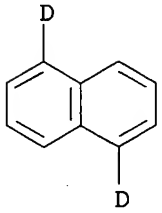
RN 19617-83-5 CAPLUS
CN Benzen-2,3,5,6-d4-amine (9CI) (CA INDEX NAME)



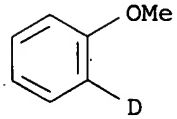
RN 20938-43-6 CAPLUS
CN Benzene-d, 4-methoxy- (9CI) (CA INDEX NAME)



RN 23878-49-1 CAPLUS
CN Naphthalene-1,5-d2 (8CI, 9CI) (CA INDEX NAME)

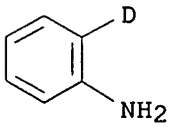


RN 26351-62-2 CAPLUS
CN Benzene-d, 2-methoxy- (9CI) (CA INDEX NAME)

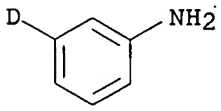


RN 50535-17-6 CAPLUS

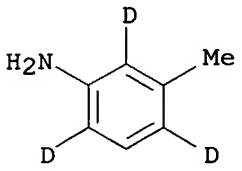
CN Benzen-2-d-amine (CA INDEX NAME)



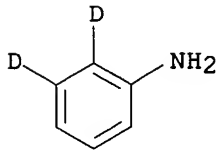
RN 50535-18-7 CAPLUS
CN Benzen-3-d-amine (9CI) (CA INDEX NAME)



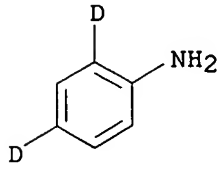
RN 68408-23-1 CAPLUS
CN Benzen-2,4,6-d3-amine, 3-methyl- (9CI) (CA INDEX NAME)



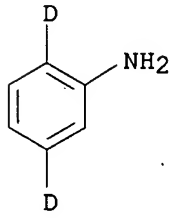
RN 120364-25-2 CAPLUS
CN Benzen-2,3-d2-amine (9CI) (CA INDEX NAME)



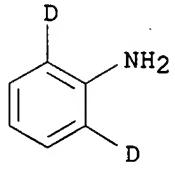
RN 122258-85-9 CAPLUS
CN Benzen-2,4-d2-amine (9CI) (CA INDEX NAME)



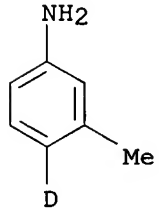
RN 129453-25-4 CAPLUS
CN Benzen-2,5-d2-amine (9CI) (CA INDEX NAME)



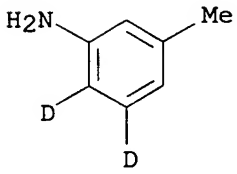
RN 129453-26-5 CAPLUS
CN Benzen-2,6-d2-amine (9CI) (CA INDEX NAME)



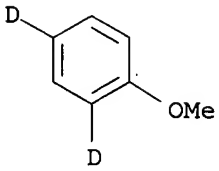
RN 129453-27-6 CAPLUS
CN Benzen-4-d-amine, 3-methyl- (9CI) (CA INDEX NAME)



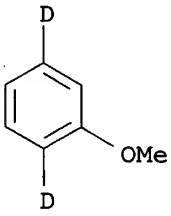
RN 129453-28-7 CAPLUS
CN Benzen-2,3-d2-amine, 5-methyl- (9CI) (CA INDEX NAME)



RN 129453-29-8 CAPLUS
CN Benzene-1,3-d2, 4-methoxy- (9CI) (CA INDEX NAME)




RN 129453-30-1 CAPLUS
CN Benzene-1,4-d2, 2-methoxy- (9CI) (CA INDEX NAME)

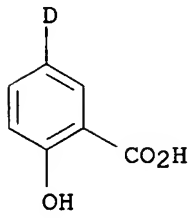



L24 ANSWER 51 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1990:197765 CAPLUS
DOCUMENT NUMBER: 112:197765
ORIGINAL REFERENCE NO.: 112:33421a,33424a
TITLE: Reductive dechlorination of chlorophenols and -benzoic acids by Raney cobalt-aluminum alloy in an alkaline deuterium oxide solution and preparation of deuterated salicylic acids
AUTHOR(S): Tashiro, Masashi; Tsuzuki, Hirohisa; Matsumoto, Junichi; Mataka, Shuntaro; Nakayama, Kouji; Tsuruta, Youichi; Yonemitsu, Tadashi
CORPORATE SOURCE: Inst. Adv. Mater. Study, Kyushu Univ., Kasuga, 816, Japan
SOURCE: Journal of Chemical Research, Synopses (1989), (12), 372-3
CODEN: JRPSDC; ISSN: 0308-2342
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 112:197765
AB Treatment of monochlorophenols or -benzoic acids with NaOD in D2O containing Raney Co-Al alloy gave the corresponding monodeuterated compds. in 86-93% isotopic purity. Di-, tri-, or tetrachloro derivs. gave the deuterated products in 70-84% isotopic purity. Chlorosalicylic acids gave the deuterio acids in 91-93% isotopic purity.
IT 11114-55-9
RL: CAT (Catalyst use); USES (Uses)
(catalysts, for reductive deuteration of chlorophenols, -benzoic acids, and -salicylic acid)
RN 11114-55-9 CAPLUS
CN Aluminum alloy, nonbase, Al,Co (CA INDEX NAME)

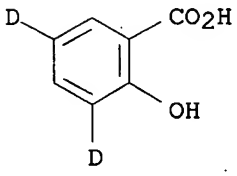
| Component | Component Registry Number |
|---|---|

Al 7429-90-5
Co 7440-48-4

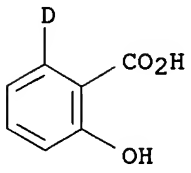
IT 32576-63-9P, 5-Deuterio-2-hydroxybenzoic acid 78617-14-8P
, 3,5-Dideuterio-2-hydroxybenzoic acid 84450-89-5P,
6-Deuterio-2-hydroxybenzoic acid 126711-92-0P,
3-Deuterio-2-hydroxybenzoic acid 126711-93-1P,
4-Deuterio-2-hydroxybenzoic acid 126711-94-2P,
3,4-Dideuterio-2-hydroxybenzoic acid 126711-95-3P,
4,5-Dideuterio-2-hydroxybenzoic acid 126711-96-4P
126711-97-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP
(Preparation); RACT (Reactant or reagent)
(preparation and acetylation of)
RN 32576-63-9 CAPLUS
CN Benzoic-3-d acid, 6-hydroxy- (9CI) (CA INDEX NAME)



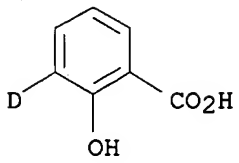

RN 78617-14-8 CAPLUS
CN Benzoic-3,5-d2 acid, 2-hydroxy- (9CI) (CA INDEX NAME)



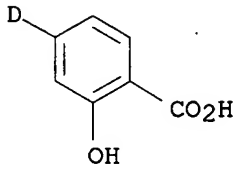

RN 84450-89-5 CAPLUS
CN Benzoic-2-d acid, 6-hydroxy- (9CI) (CA INDEX NAME)



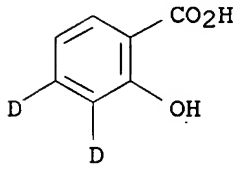

RN 126711-92-0 CAPLUS
CN Benzoic-3-d acid, 2-hydroxy- (9CI) (CA INDEX NAME)



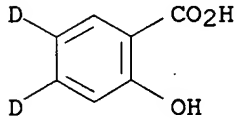
RN 126711-93-1 CAPLUS
CN Benzoic-4-d acid, 2-hydroxy- (9CI) (CA INDEX NAME)



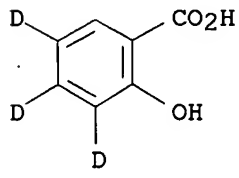
RN 126711-94-2 CAPLUS
CN Benzoic-3,4-d2 acid, 2-hydroxy- (9CI) (CA INDEX NAME)



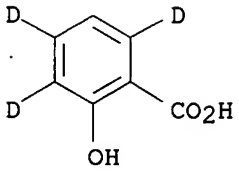
RN 126711-95-3 CAPLUS
CN Benzoic-4,5-d2 acid, 2-hydroxy- (9CI) (CA INDEX NAME)



RN 126711-96-4 CAPLUS
CN Benzoic-3,4,5-d3 acid, 2-hydroxy- (9CI) (CA INDEX NAME)

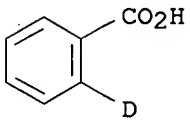


RN 126711-97-5 CAPLUS
CN Benzoic-2,4,5-d3 acid, 6-hydroxy- (9CI) (CA INDEX NAME)

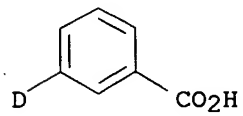


IT 4551-39-7P, 2-Deuteriobenzoic acid 4551-61-5P, 3-Deuteriobenzoic acid 4551-62-6P, 4-Deuteriobenzoic acid 4551-63-7P, 2,3-Dideuteriobenzoic acid 14435-76-8P, 2,4,6-Trideuteriobenzoic acid 23951-01-1P, 2-Deuteriophenol 23951-02-2P, 3-Deuteriophenol 23951-03-3P, 4-Deuteriophenol 37960-84-2P, 3,5-Dideuteriobenzoic acid 52199-97-0P, 3,4-Dideuteriobenzoic acid 57193-23-4P, 2,4-Dideuteriobenzoic acid 64045-84-7P, 2,3,4,6-Tetradeuteriophenol 64045-89-2P, 2,4-Dideuteriophenol 87976-29-2P, 2,3,5-Trideuteriobenzoic acid 87976-30-5P, 2,4,5-Trideuteriobenzoic acid 87976-34-9P, 2,3,4,5-Tetradeuteriobenzoic acid 126711-90-8P, 3,4,5-Trideuteriophenol 126711-98-6P 126711-99-7P 126712-00-3P 126712-01-4P 126735-99-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

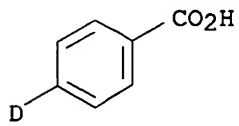
RN 4551-39-7 CAPLUS
CN Benzoic-2-d acid (9CI) (CA INDEX NAME)



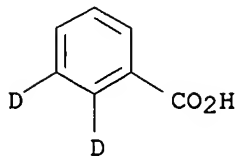
RN 4551-61-5 CAPLUS
CN Benzoic-3-d acid (9CI) (CA INDEX NAME)



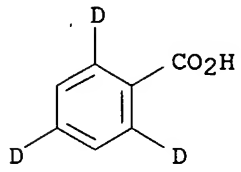
RN 4551-62-6 CAPLUS
CN Benzoic-4-d acid (CA INDEX NAME)



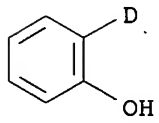
RN 4551-63-7 CAPLUS
CN Benzoic-2,3-d2 acid (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



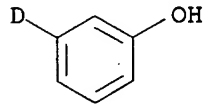
RN 14435-76-8 CAPLUS
CN Benzoic-2,4,6-d3 acid (7CI, 8CI, 9CI) (CA INDEX NAME)



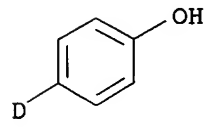
RN 23951-01-1 CAPLUS
CN Phen-2-d-ol (9CI) (CA INDEX NAME)



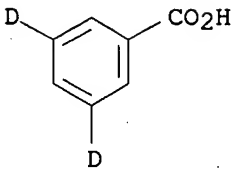
RN 23951-02-2 CAPLUS
CN Phen-3-d-ol (9CI) (CA INDEX NAME)



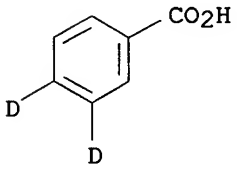
RN 23951-03-3 CAPLUS
CN Phen-4-d-ol (CA INDEX NAME)



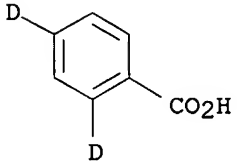
RN 37960-84-2 CAPLUS
CN Benzoic-3,5-d2 acid (CA INDEX NAME)



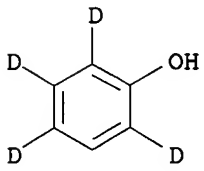
RN 52199-97-0 CAPLUS
CN Benzoic-3,4-d2 acid (9CI) (CA INDEX NAME)



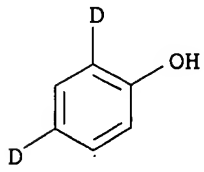
RN 57193-23-4 CAPLUS
CN Benzoic-2,4-d2 acid (9CI) (CA INDEX NAME)



RN 64045-84-7 CAPLUS
CN Phen-2,3,4,6-d4-ol (9CI) (CA INDEX NAME)

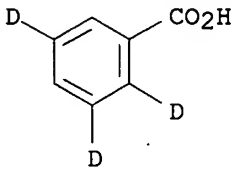


RN 64045-89-2 CAPLUS
CN Phen-2,4-d2-ol (9CI) (CA INDEX NAME)

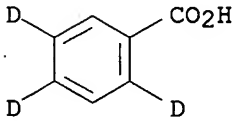


RN 87976-29-2 CAPLUS

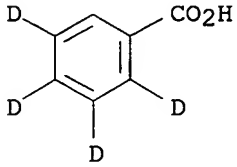
CN Benzoic-2,3,5-d3 acid (9CI) (CA INDEX NAME)



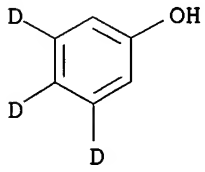
RN 87976-30-5 CAPLUS
CN Benzoic-2,4,5-d3 acid (9CI) (CA INDEX NAME)



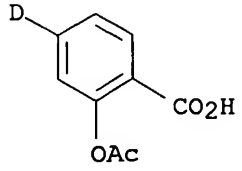
RN 87976-34-9 CAPLUS
CN Benzoic-2,3,4,5-d4 acid (9CI) (CA INDEX NAME)



RN 126711-90-8 CAPLUS
CN Phen-3,4,5-d3-ol (9CI) (CA INDEX NAME)

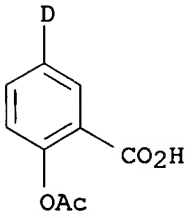


RN 126711-98-6 CAPLUS
CN Benzoic-4-d acid, 2-(acetyloxy)- (9CI) (CA INDEX NAME)

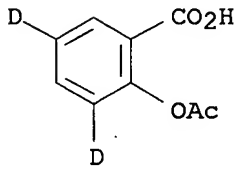


RN 126711-99-7 CAPLUS

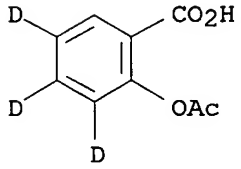
CN Benzoic-3-d acid, 6-(acetyloxy)- (9CI) (CA INDEX NAME)



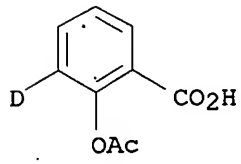
RN 126712-00-3 CAPLUS
CN Benzoic-3,5-d2 acid, 2-(acetyloxy)- (9CI) (CA INDEX NAME)



RN 126712-01-4 CAPLUS
CN Benzoic-3,4,5-d3 acid, 2-(acetyloxy)- (9CI) (CA INDEX NAME)

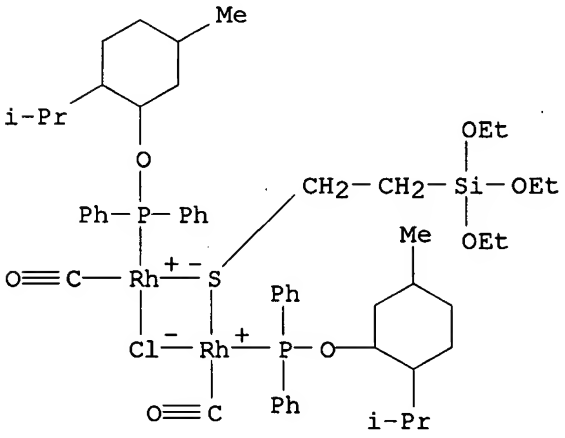


RN 126735-99-7 CAPLUS
CN Benzoic-3-d acid, 2-(acetyloxy)- (9CI) (CA INDEX NAME)

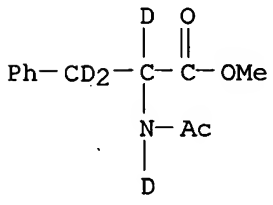


L24 ANSWER 52 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1989:515723 CAPLUS
DOCUMENT NUMBER: 111:115723
ORIGINAL REFERENCE NO.: 111:19415a,19418a
TITLE: Evidence for exchange processes associated with the hydrogenation of methyl (Z)-α-acetamidocinnamate by a silica-bound chiral dirhodium catalyst
AUTHOR(S): Eisen, Moris; Blum, Jochanan; Hoehne, Gerhard;

Schumann, Herbert; Schwarz, Helmut
CORPORATE SOURCE: Dep. Org. Chem., Hebrew Univ., Jerusalem, 91904, Israel
SOURCE: Chemische Berichte (1989), 122(8), 1599-601
CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 111:115723
AB Mass spectral anal. showed that H-D exchange took place during the deuteration of (Z)-PhCH:C(NHAc)CO2Me by D2 in MeOH/C6H6 or CD3OD/C6H6 catalyzed by a silica-bound chiral dirhodium phosphine complex.
IT 121314-63-4D, silica-bound
RL: CAT (Catalyst use); USES (Uses)
(catalyst, for hydrogenation and deuteration of Me acetamidocinnamate)
RN 121314-63-4 CAPLUS
CN Rhodium, dicarbonyl-μ-chlorobis[5-methyl-2-(1-methylethyl)cyclohexyl diphenylphosphinite-P][μ-[2-(triethoxysilyl)ethanethiolato-S:S]]di-, stereoisomer (9CI) (CA INDEX NAME)



IT 121314-62-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by deuteration of Me acetamidocinnamate catalyzed by silica-bound chiral dirhodium complex)
RN 121314-62-3 CAPLUS
CN Phenylalanine-N,α,β,β-d4, N-acetyl-, methyl ester (9CI) (CA INDEX NAME)

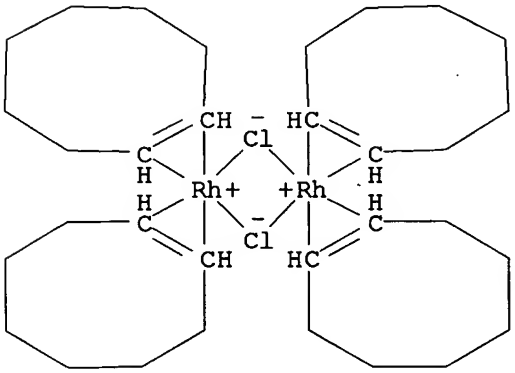


L24 ANSWER 53 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1989:231056 CAPLUS

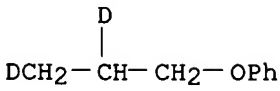
DOCUMENT NUMBER: 110:231056
ORIGINAL REFERENCE NO.: 110:38287a,38290a
TITLE: Homogeneous deuteration of alkenes using [RhCl(4R,5R-diop)] catalysts
AUTHOR(S): Gungor, Muammer; Jardine, Fred H.; Wheatley, J. Denis
CORPORATE SOURCE: Dep. Phys. Sci., North East London Polytech., London, E15 4LZ, UK
SOURCE: Polyhedron (1988), 7(19-20), 1827-9
CODEN: PLYHDE; ISSN: 0277-5387
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Mass spectrometric analyses of the products from the homogeneous deuteration of alkenes using the title (4R,5R-DIOP)/{[RhCl(cyclooctene)2]2} catalyst system show that considerable quantities of polydeuterated products are obtained. These products arise from the decomposition of the intermediate rhodium(III)alkyl complex [RhDCl(alkyl)(DIOP)] before the second atom of deuterium can be transferred to the alkyl ligand. Its decomposition by β-hydride abstraction brings about both polydeuteration and scrambled addition of deuterium to the alkene. The yields of specifically deuterated products are inferior to those obtained from Wilkinson-type catalysts. The best yields of dideuterated products are obtained from substituted alkenes that chelate to the catalyst and thereby stabilize the intermediate alkyl. The preparation of a threitol ditosylate intermediate in dry pyridine was noted for its dangerous exothermicity.

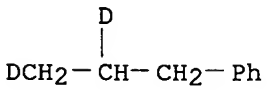
IT 12279-09-3
RL: CAT (Catalyst use); USES (Uses)
(catalysts, containing DIOP, for deuteration of alkenes)
RN 12279-09-3 CAPLUS
CN Rhodium, di-μ-chlorotetrakis[(1,2-η)-cyclooctene]di- (CA INDEX NAME)



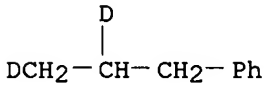

IT 73811-48-0P 118297-06-6P 118297-07-7P
120626-02-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 73811-48-0 CAPLUS
CN Benzene, propoxy-2,3-d2- (9CI) (CA INDEX NAME)



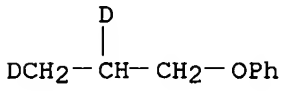
RN 118297-06-6 CAPLUS
CN Benzene, propyl-2,3-d2- (9CI) (CA INDEX NAME)



RN 118297-07-7 CAPLUS
CN Benzene, propyl-2,3-d2-, labeled with deuterium (9CI) (CA INDEX NAME)



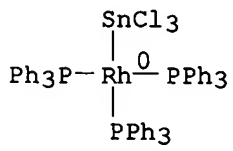
RN 120626-02-0 CAPLUS
CN Benzene, (propoxy-2,3,?-d3)- (9CI) (CA INDEX NAME)



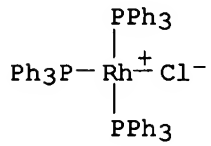
L24 ANSWER 54 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1989:94278 CAPLUS
DOCUMENT NUMBER: 110:94278
ORIGINAL REFERENCE NO.: 110:15567a,15570a
TITLE: Homogeneous deuteriation of alkenes using halotris(triarylphosphine)rhodium catalysts
AUTHOR(S): Gungor, Muammer; Jardine, Fred H.; Wheatley, J. Denis
CORPORATE SOURCE: Dep. Phys. Sci., North East London Polytech., London, E15 4LZ, UK
SOURCE: Journal of the Chemical Society, Dalton Transactions: Inorganic Chemistry (1972-1999) (1988), (6), 1653-6
CODEN: JCDTBI; ISSN: 0300-9246
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 110:94278
AB Catalytic deuteriation of cycloalkenes using RhX(PR3)3 (X = halide, R = aryl) catalysts frequently gives rise to polydeuteriation and scrambled addition of deuterium to the cycloalkene substrate. These undesirable side reactions can be minimized by using small, electroneg. aniono ligands or electron-withdrawing triarylphosphine ligands. Both these ligands inhibit the decomposition of the 16-electron intermediate rhodium(III) alkyl complex RhD(X)alkyl)(PR3)2. Its decomposition by β-hydride abstraction brings about both polydeuteriation and scrambled addition of deuterium to the alkenes. Acyclic, alk-1-enes give the best yields of [2H2] products when

RhI(PPh3)3 is the catalyst, since the formation of the less stable 2-alkyl intermediate is sterically inhibited.

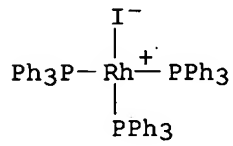
IT 19584-17-9
RL: CAT (Catalyst use); USES (Uses)
(catalysts, for deuteriation of cyclooctene)
RN 19584-17-9 CAPLUS
CN Rhodium, (trichlorostannyl)tris(triphenylphosphine)-, (SP-4-2)- (CA INDEX NAME)



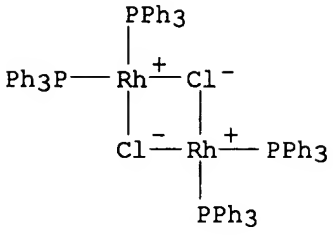
IT 14694-95-2 14973-90-1
RL: CAT (Catalyst use); USES (Uses)
(catalysts, for homogeneous deuteriation of alkenes)
RN 14694-95-2 CAPLUS
CN Rhodium, chlorotris(triphenylphosphine)-, (SP-4-2)- (CA INDEX NAME)



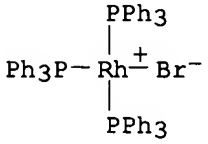
RN 14973-90-1 CAPLUS
CN Rhodium, iodotris(triphenylphosphine)-, (SP-4-2)- (CA INDEX NAME)



IT 14653-50-0 14973-89-8 25478-56-2
119029-03-7
RL: CAT (Catalyst use); USES (Uses)
(catalysts, for polydeuteriation of alkenes)
RN 14653-50-0 CAPLUS
CN Rhodium, di-μ-chlorotetrakis(triphenylphosphine)di- (CA INDEX NAME)



RN 14973-89-8 CAPLUS
CN Rhodium, bromotris(triphenylphosphine)-, (SP-4-2)- (CA INDEX NAME)



RN 25478-56-2 CAPLUS
CN Rhodium, chlorotris[tris(4-fluorophenyl)phosphine-κP]-, (SP-4-2)-
(CA INDEX NAME)

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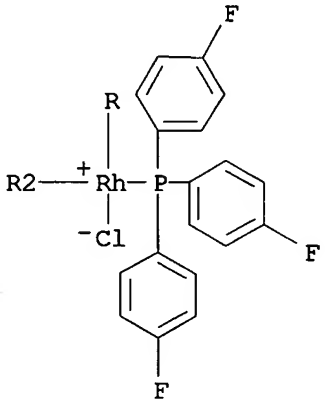

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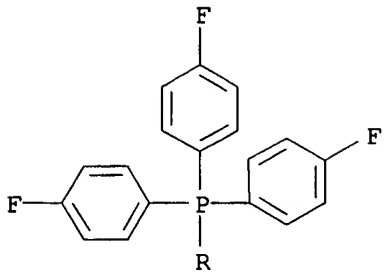


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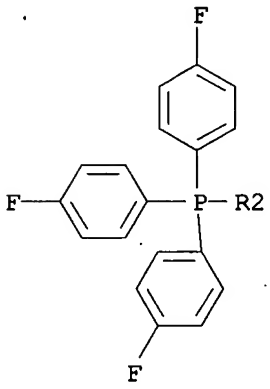
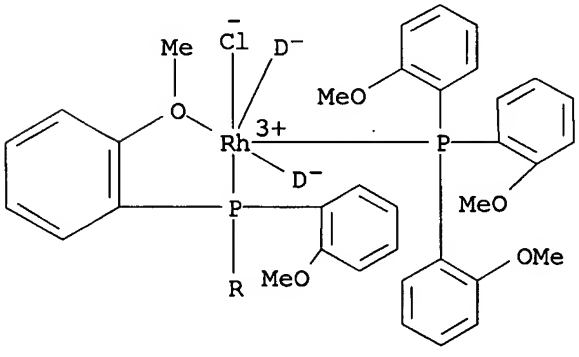
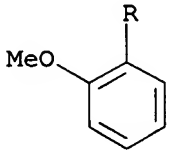
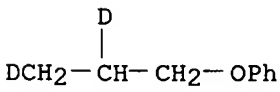



RN 119029-03-7 CAPLUS
CN Rhodium, chlorodihydro-d2-[tris(2-methoxyphenyl)phosphine-O,P][tris(2-methoxyphenyl)phosphine-P]- (9CI) (CA INDEX NAME)

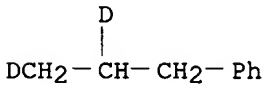


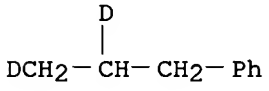
IT 73811-48-0P 118297-06-6P 118297-07-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 73811-48-0 CAPLUS
CN Benzene, propoxy-2,3-d2- (9CI) (CA INDEX NAME)



RN 118297-06-6 CAPLUS
CN Benzene, propyl-2,3-d2- (9CI) (CA INDEX NAME)



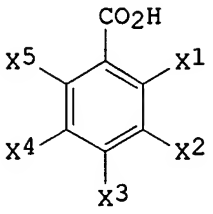
RN 118297-07-7 CAPLUS
CN Benzene, propyl-2,3-d2-, labeled with deuterium (9CI) (CA INDEX NAME)



L24 ANSWER 55 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1988:510031 CAPLUS
DOCUMENT NUMBER: 109:110031
ORIGINAL REFERENCE NO.: 109:18319a,18322a
TITLE: Preparation of deuterated benzoic acids as labeled intermediates for pharmaceuticals, agrochemicals, and perfumes
INVENTOR(S): Tashiro, Masashi; Nakayama, Mitsuharu; Yonemitsu, Naoshi; Matsumoto, Junichi
PATENT ASSIGNEE(S): Unitika Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 3 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| JP 63030450 | A | 19880209 | JP 1986-176450 | 19860724 |
| JP 05075734 | B | 19931021 | | |
| PRIORITY APPLN. INFO.: | | | JP 1986-176450 | 19860724 |

OTHER SOURCE(S): MARPAT 109:110031
GI



I

AB The title labeled compds. (I; X1-5 = H, D) (II), useful as intermediates in studying pharmaceuticals, agrochems., and perfumes, are prepared 2-ClC6H4CO2H in 10% NaOD-D2O was stirred at 70° in the presence of a Raney Co-Al alloy to give 90% PhCO2H-2-D.

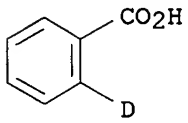
IT 11114-55-9
RL: CAT (Catalyst use); USES (Uses)
(catalyst, for deuteration of chlorobenzoic acids)

RN 11114-55-9 CAPLUS
CN Aluminum alloy, nonbase, Al,Co (CA INDEX NAME)

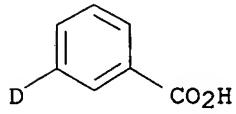
| Component | Component Registry Number |
|---|---|
| Al | 7429-90-5 |
| Co | 7440-48-4 |

IT 4551-39-7P 4551-61-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for pharmaceuticals, agrochems., and perfumes)

RN 4551-39-7 CAPLUS
CN Benzoic-2-d acid (9CI) (CA INDEX NAME)



RN 4551-61-5 CAPLUS
CN Benzoic-3-d acid (9CI) (CA INDEX NAME)

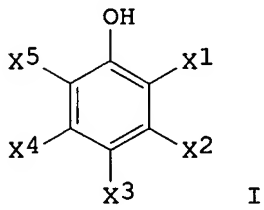


L24 ANSWER 56 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1988:510013 CAPLUS
DOCUMENT NUMBER: 109:110013
ORIGINAL REFERENCE NO.: 109:18315a,18318a
TITLE: Preparation of deuterated phenols as labeled intermediates for pharmaceuticals, agrochemicals, and perfumes

INVENTOR(S): Tashiro, Masashi; Nakayama, Mitsuharu; Yonemitsu, Naoshi; Matsumoto, Junichi
PATENT ASSIGNEE(S): Unitika Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 3 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| JP 63030435 | A | 19880209 | JP 1986-176451 | 19860724 |
| JP 06053693 | B | 19940720 | | |

PRIORITY APPLN. INFO.: JP 1986-176451 19860724
OTHER SOURCE(S): MARPAT 109:110013
GI



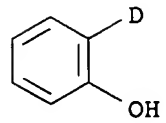

I

AB The title labeled compds. (I; X1-5 = H, D) (II), useful as intermediates in studying pharmaceuticals, agrochems., and perfumes, are prepared 2-ClC6H4OH in 10% NaOD-D2O was stirred at 70° in the presence of a Raney Co-Al alloy to give 70% PhOH-2-D.

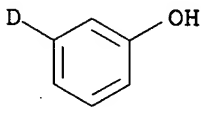
IT 11114-55-9
RL: CAT (Catalyst use); USES (Uses)
(catalyst, for deuteration of chlorophenols)
RN 11114-55-9 CAPLUS
CN Aluminum alloy, nonbase, Al,Co (CA INDEX NAME)

| Component | Component Registry Number |
|---|---|
| Al | 7429-90-5 |
| Co | 7440-48-4 |

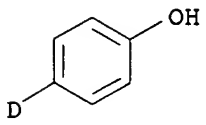
IT 23951-01-1P 23951-02-2P 23951-03-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for pharmaceuticals, agrochems. and perfumes)
RN 23951-01-1 CAPLUS
CN Phen-2-d-ol (9CI) (CA INDEX NAME)



RN 23951-02-2 CAPLUS
CN Phen-3-d-ol (9CI) (CA INDEX NAME)



RN 23951-03-3 CAPLUS
CN Phen-4-d-ol (CA INDEX NAME)



L24 ANSWER 57 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1988:493813 CAPLUS
DOCUMENT NUMBER: 109:93813
ORIGINAL REFERENCE NO.: 109:15679a,15682a
TITLE: Preparation of 2,2-bis(4-hydroxy-2,6-dideuteriophenyl)propane
INVENTOR(S): Tashiro, Masashi; Nishinohara, Minoru; Okuda, Kazuhide
PATENT ASSIGNEE(S): Unitika Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 3 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| JP 63030439 | A | 19880209 | JP 1986-176449 | 19860724 |
| JP 06057665 | B | 19940803 | | |

PRIORITY APPLN. INFO.: JP 1986-176449 19860724

AB The title compound (I), which is useful as a material for light- and oxidation-resistant polycarbonates, polyesters, and phenolic resins with improved near-IR permeability, is prepared by treating 2,2-bis(4-hydroxyphenyl)propane (II) with Raney Ni alloys in D2O containing alkali erosive agents. II (1.14 g) was mixed with 1.5 g Raney Ni-Al alloy in D2O containing 10% NaOD under N and the mixture was stirred 5 h at 100° to give 1.10 g I.

IT 7440-02-0, Nickel, uses and miscellaneous
RL: CAT (Catalyst use); USES (Uses)
(catalysts, alloys, deuteration of bisphenol A in presence of)

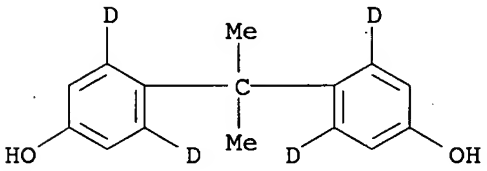
RN 7440-02-0 CAPLUS
CN Nickel (CA INDEX NAME)

Ni

IT 11114-68-4
RL: CAT (Catalyst use); USES (Uses)
(catalysts, deuteration of bisphenol A in presence of)
RN 11114-68-4 CAPLUS
CN Aluminum alloy, nonbase, Al,Ni (CA INDEX NAME)

| Component | Component Registry Number |
|---|---|
| Al | 7429-90-5 |
| Ni | 7440-02-0 |

IT 102438-62-0P
RL: PREP (Preparation)
(preparation of, as material for heat- and oxidation-resistant polymers with improved near-IR transparency)
RN 102438-62-0 CAPLUS
CN Phen-3,5-d2-ol, 4,4'-(1-methylethylidene)bis- (9CI) (CA INDEX NAME)



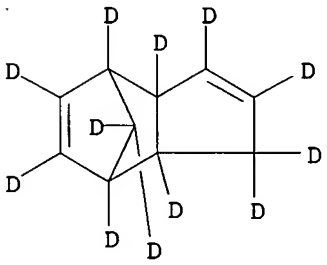

L24 ANSWER 58 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1988:186970 CAPLUS
DOCUMENT NUMBER: 108:186970
ORIGINAL REFERENCE NO.: 108:30727a,30730a
TITLE: Deuterium-labeling experiments relevant to the mechanism of platinum-catalyzed hydrogenation of (diolefin)dialkylplatinum(II) complexes: evidence for isotopic exchange via platinum surface hydrogen. The stereochemistry of reduction
AUTHOR(S): Miller, Timothy M.; McCarthy, Thomas J.; Whitesides, George M.
CORPORATE SOURCE: Dep. Chem., Harvard Univ., Cambridge, MA, 02138, USA
SOURCE: Journal of the American Chemical Society (1988), 110(10), 3156-63
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 108:186970
AB Reduction of (diolefin)dialkylplatinum(II) complexes with H2 over a platinum black catalyst is accompanied by interchange of H among the organic groups and gaseous H2. Exchange of H between an alkane solvent and these organic groups also occurs during the reaction, but only relatively slowly. An examination of the stereochem. of reduction of (norbornadiene)dimethylplatinum(II) with D2 indicates that the D atoms add predominantly to the same (endo) face of the olefins as that coordinated to the dimethylplatinum moiety. Reduction of uncomplicated norbornadiene under the same conditions yields norborane having primarily exo C-D bonds. These expts. are compatible

with a mechanism for the reduction involving adsorption of the (diolefin)dialkylplatinum(II) complex on the surface of the Pt catalyst via its Pt atom, conversion of the organic moieties of the soluble (diolefin)dialkylplatinum complex to Pt-surface alkyls, and interchange of H atoms between these surface alkyls via a mobile pool of Pt-surface H atoms. Combination of the surface alkyls with surface H yields alkanes in a final irreversible step. Comparison of the evidence from D-interchange expts. conducted under mass transport limited and reaction rate limited conditions is consistent with the hypothesis that the concentration of H on the Pt surface is lower under mass transport limited conditions.

IT 7440-06-4, Platinum, uses and miscellaneous
RL: CAT (Catalyst use); USES (Uses)
(catalyst, for hydrogenation of diolefindialkylplatinum complex, mechanism in relation to)
RN 7440-06-4 CAPLUS
CN Platinum (CA INDEX NAME)

Pt

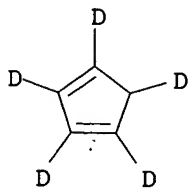
IT 65886-42-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and complexation of, with platinum chloride)
RN 65886-42-2 CAPLUS
CN 4,7-Methano-1H-indene-1,1,2,3,5,6,8,8-d8, 3a,4,7,7a-tetrahydro-d4- (9CI) (CA INDEX NAME)



IT 113507-24-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and deuteration of)
RN 113507-24-7 CAPLUS
CN 1,3-Cyclopentadiene-d4 (9CI) (CA INDEX NAME)

IT 16456-47-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and dimerization of)
RN 16456-47-6 CAPLUS

CN 1,3-Cyclopentadiene-1,2,3,4,5-d5 (8CI, 9CI) (CA INDEX NAME)




IT 113490-41-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and methylation of)
RN 113490-41-8 CAPLUS
CN Platinum, dichloro[(2,3,5,6-η)-3a,4,7,7a-tetrahydro-d4-4,7-methano-1H-indene-1,1,2,3,5,6,8,8-d8]- (9CI) (CA INDEX NAME)

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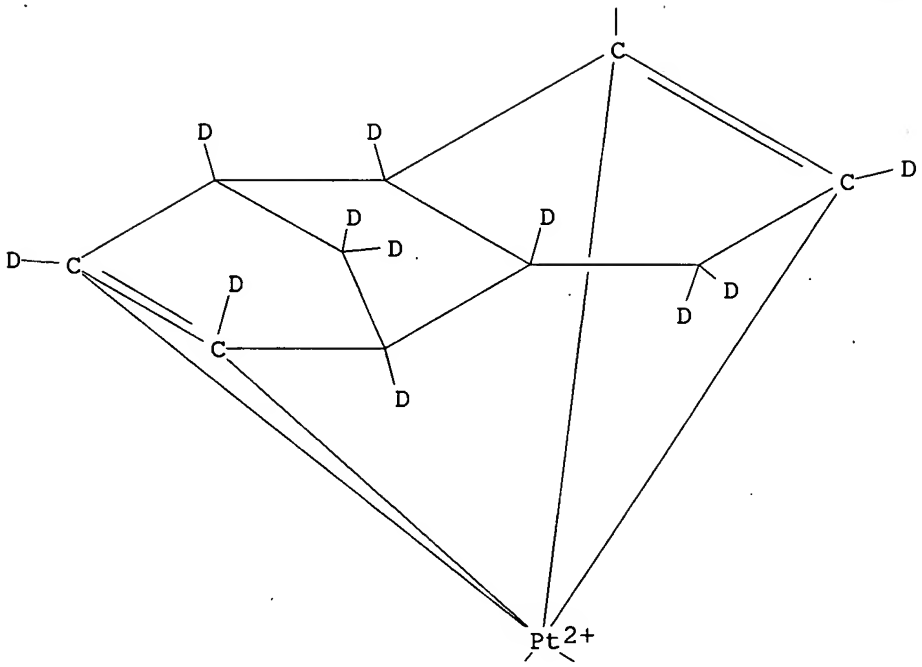
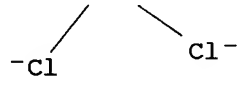



PAGE 3-A




IT 113490-40-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and platinum-catalyzed hydrogenation of, mechanism of)
RN 113490-40-7 CAPLUS
CN Platinum, dimethyl[(2,3,5,6-η)-3a,4,7,7a-tetrahydro-d4-4,7-methano-1H-indene-1,1,2,3,5,6,8,8-d8]- (9CI) (CA INDEX NAME)

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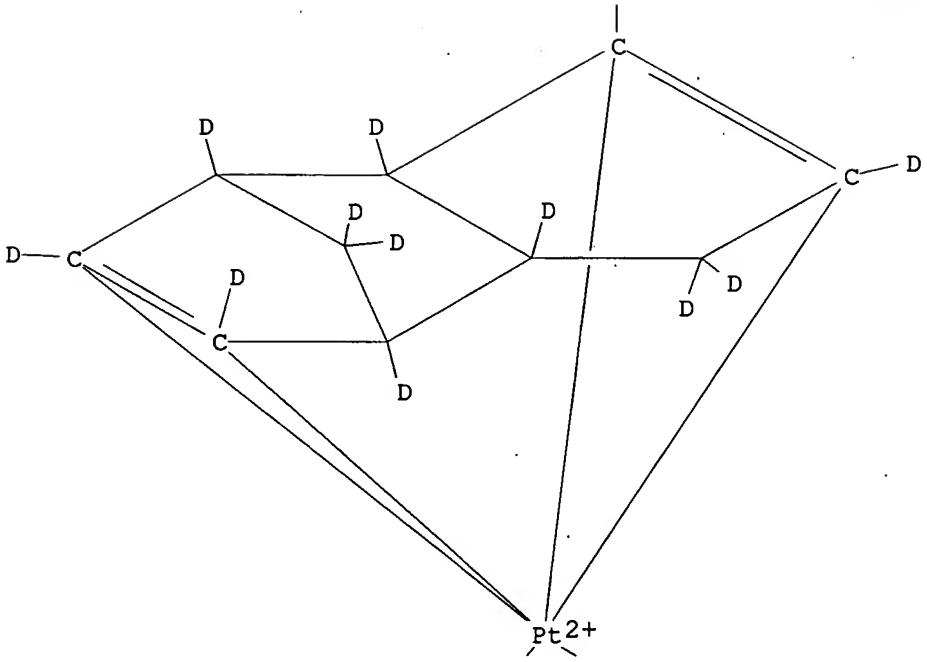

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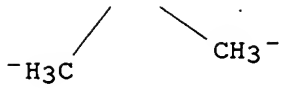
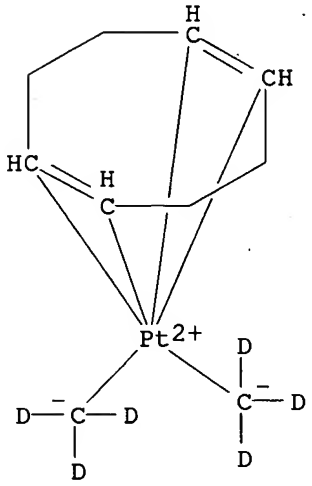


IT 113451-87-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and platinum-catalyzed hydrogenation of, with deuterium-labeling, mechanism of)
RN 113451-87-9 CAPLUS
CN Platinum, [(1,2,5,6-η)-1,5-cyclooctadiene]di(methyl-d3)- (9CI) (CA INDEX NAME)



L24 ANSWER 59 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1988:38451 CAPLUS
DOCUMENT NUMBER: 108:38451
ORIGINAL REFERENCE NO.: 108:6455a,6458a
TITLE: Selectivity during hydrogenation of phenylacetylene on metallic catalysts
AUTHOR(S): Sokol'skii, D. V.; Ualikhanova, A.; Korolev, A. V.
CORPORATE SOURCE: Inst. Org. Katal. Elektrokhim., Alma-Ata, USSR
SOURCE: Izvestiya Akademii Nauk Kazakhskoi SSR, Seriya Khimicheskaya (1987), (5), 32-5
CODEN: IKAKAK; ISSN: 0002-3205
DOCUMENT TYPE: Journal
LANGUAGE: Russian
AB In the partial hydrogenation of phenylacetylene (I) to styrene at 286-323 K in the presence of Pt, Pd, Rh, Fe, Co, and Ni catalysts, the selectivity of hydrogenation increased for all catalysts on replacing I with monodeuterated I. A linear dependence was observed between selectivity of hydrogenation and the concentration of cis-PhCH:CDH.
IT 7440-02-0, Nickel, uses and miscellaneous 7440-06-4, Platinum, uses and miscellaneous 7440-16-6, Rhodium, uses and miscellaneous 7440-48-4, Cobalt, uses and miscellaneous
RL: CAT (Catalyst use); USES (Uses)

(catalysts, for hydrogenation of phenylacetylene to styrene, deuteration effect on selectivity of)
RN 7440-02-0 CAPLUS
CN Nickel (CA INDEX NAME)

Ni

RN 7440-06-4 CAPLUS
CN Platinum (CA INDEX NAME)

Pt

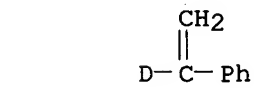
RN 7440-16-6 CAPLUS
CN Rhodium (CA INDEX NAME)

Rh

RN 7440-48-4 CAPLUS
CN Cobalt (CA INDEX NAME)

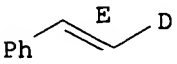
Co

IT 1193-80-2P, α-Deuterostyrene 6911-81-5P, β-trans-Deuterostyrene 21370-59-2P, β-cis-Deuterostyrene
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in hydrogenation of monodeuterophenylacetylene)
RN 1193-80-2 CAPLUS
CN Benzene, ethenyl-1-d- (9CI) (CA INDEX NAME)



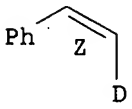
RN 6911-81-5 CAPLUS
CN Benzene, (1E)-ethenyl-2-d- (CA INDEX NAME)

Double bond geometry as shown.



RN 21370-59-2 CAPLUS
CN Benzene, (1Z)-ethenyl-2-d- (CA INDEX NAME)

Double bond geometry as shown.

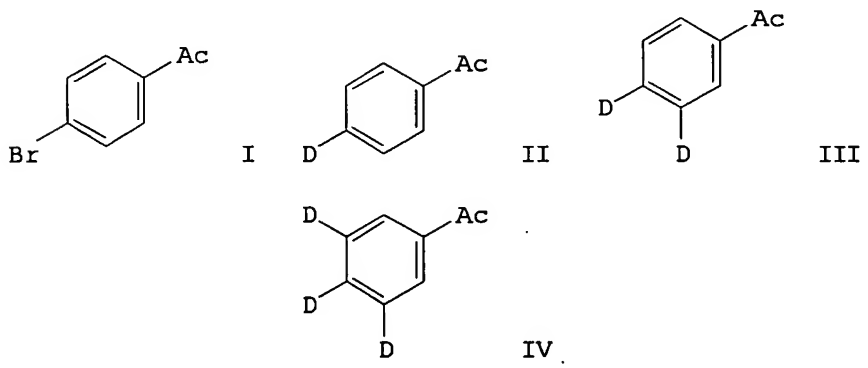


IT 3240-11-7, Monodeuterophenylacetylene
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrogenation of, to styrene, in presence of metal catalysts, selectivity in)
RN 3240-11-7 CAPLUS
CN Benzene, ethynyl-d- (CA INDEX NAME)

L24 ANSWER 60 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1986:533517 CAPLUS
DOCUMENT NUMBER: 105:133517
ORIGINAL REFERENCE NO.: 105:21533a,21536a
TITLE: Highly selective introduction of hydrogen isotopes into aromatic compounds
INVENTOR(S): Tashiro, Masashi; Nakayama, Mitsuharu; Nakamura, Hiroshi; Aoki, Yuichi; Takigawa, Akio; Maeda, Koichi; Tago, Ikuo; Yoshida, Motoaki
PATENT ASSIGNEE(S): Nippon Sheet Glass Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 3 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|---|---|---|---|
| JP 61053228 | A | 19860317 | JP 1984-174767 | 19840822 |
| JP 05017894 | B | 19930310 | | |
| PRIORITY APPLN. INFO.: | | | JP 1984-174767 | 19840822 |

OTHER SOURCE(S): CASREACT 105:133517
GI



I II III IV

AB Aromatic compds. were deuterated or tritiated with high selectivity by reaction of halo aromatic compds. with aqueous alkali solution containing the H isotope over Raney metal catalysts under ultrasound. Thus, Raney Ni-Al alloy was added to a solution of I in NaOD-D2O and the mixture stirred at 50-60° to give II 19, III 29, and IV 31%, vs. 83% II alone when using ultrasound.

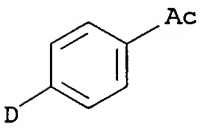
IT 11114-68-4
RL: CAT (Catalyst use); USES (Uses)
(catalysts, for deuteration of bromoacetophenone)

RN 11114-68-4 CAPLUS
CN Aluminum alloy, nonbase, Al,Ni (CA INDEX NAME)

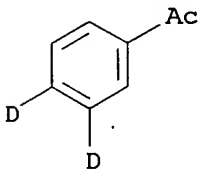
| Component | Component Registry Number |
|---|---|
| Al | 7429-90-5 |
| Ni | 7440-02-0 |

IT 72302-32-0P 104385-13-9P 104385-14-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

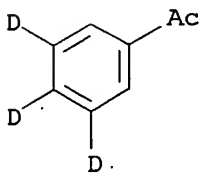
RN 72302-32-0 CAPLUS
CN Ethanone, 1-(phenyl-4-d)- (CA INDEX NAME)




RN 104385-13-9 CAPLUS
CN Ethanone, 1-(phenyl-3,4-d2)- (9CI) (CA INDEX NAME)

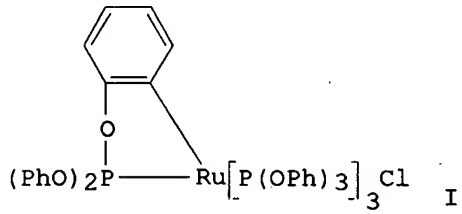



RN 104385-14-0 CAPLUS
CN Ethanone, 1-(phenyl-3,4,5-d3)- (9CI) (CA INDEX NAME)




L24 ANSWER 61 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1986:6009 CAPLUS
DOCUMENT NUMBER: 104:6009
ORIGINAL REFERENCE NO.: 104:1103a,1106a
TITLE: Reexamination of the deuteration of phenol catalyzed by an orthometalated ruthenium complex
AUTHOR(S): Lewis, Larry N.
CORPORATE SOURCE: Corp. Res. Dev. Cent., Gen. Electr. Co., Schenectady, NY, 12301, USA
SOURCE: Inorganic Chemistry (1985), 24(25), 4433-5
CODEN: INOCAJ; ISSN: 0020-1669
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 104:6009
GI

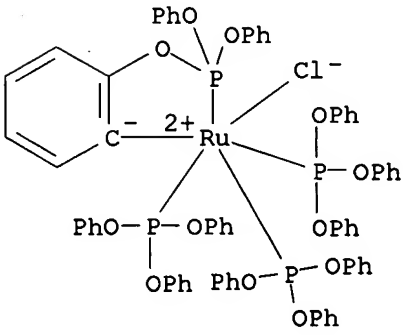



I

AB The reaction of the ortho-metalated Ru phosphite complex (I) with D2 in the presence of PhOH was reexamd. Deuterium incorporation in I was confirmed. PhOH orthodeuteration occurred in the KOPh-PhOH-I system, but not in the PhOH-I system. Thus, KOPh catalyzed the exchange reaction between PhOH and free deuterated P(OPh)3. The reaction of I with P(OC6H4Me)3 showed phosphite exchange.

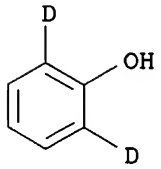
IT 25839-18-3
RL: CAT (Catalyst use); USES (Uses)
(catalyst, in ortho deuteration of phenol, mechanism in)

RN 25839-18-3 CAPLUS
CN Ruthenium, chloro[2-[(diphenoxyphosphino)oxy]phenyl-C,P]tris(triphenyl phosphite-P)-, (OC-6-24)- (9CI) (CA INDEX NAME)




IT 64045-88-1P

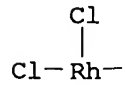
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, ruthenium phosphite catalyst in, mechanism of)
RN 64045-88-1 CAPLUS
CN Phen-2,6-d2-ol (CA INDEX NAME)



L24 ANSWER 62 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1985:560184 CAPLUS
DOCUMENT NUMBER: 103:160184
ORIGINAL REFERENCE NO.: 103:25701a,25704a
TITLE: Regioselective labeling of anilides with deuterium
AUTHOR(S): Lockley, W. J. S.
CORPORATE SOURCE: Dep. Metab. Stud., Fisons PLC, Loughborough/Leicestershire, LE11 0QY, UK
SOURCE: Journal of Labelled Compounds and Radiopharmaceuticals (1985), 22(6), 623-30
CODEN: JLCRD4; ISSN: 0362-4803
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 103:160184
AB N-Aryl amides may be deuterated by exchange with D2O in the presence of RhCl3. Under such conditions deuterium is introduced into positions ortho to the anilide N atom with a high degree of regioselectivity.
IT 7440-16-6, uses and miscellaneous 10049-07-7
RL: CAT (Catalyst use); USES (Uses)
(catalysts, for deuteration of anilide derivs. with deuterium oxide)
RN 7440-16-6 CAPLUS
CN Rhodium (CA INDEX NAME)

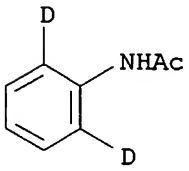
Rh

RN 10049-07-7 CAPLUS
CN Rhodium chloride (RhCl3) (CA INDEX NAME)

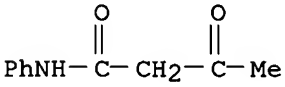


IT 26502-21-6P 98624-45-4P 98624-46-5P
98624-47-6P 98624-48-7P 98624-49-8P
98624-50-1P 98624-51-2P 98624-52-3P
98624-53-4P 98624-54-5P 98624-55-6P
98624-56-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

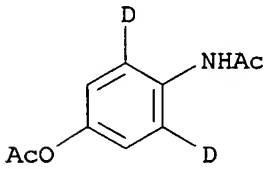
RN 26502-21-6 CAPLUS
CN Acetamide, N-(phenyl-2,6-d2)- (CA INDEX NAME)



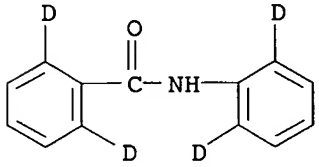
RN 98624-45-4 CAPLUS
CN Butanamide, 3-oxo-N-phenyl-, labeled with deuterium (9CI) (CA INDEX NAME)



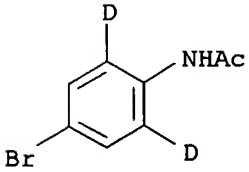
RN 98624-46-5 CAPLUS
CN Acetamide, N-[4-(acetyloxy)phenyl-2,6-d2]- (9CI) (CA INDEX NAME)



RN 98624-47-6 CAPLUS
CN Benzamide-2,6-d2, N-(phenyl-2,6-d2)- (CA INDEX NAME)

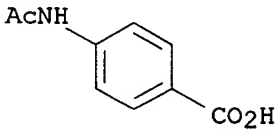


RN 98624-48-7 CAPLUS
CN Acetamide, N-(4-bromophenyl-2,6-d2)- (9CI) (CA INDEX NAME)

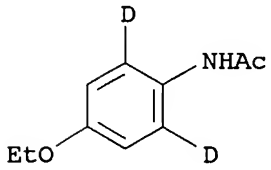


RN 98624-49-8 CAPLUS

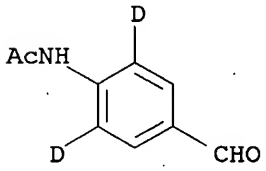
CN Benzoic acid, 4-(acetylamino)-, labeled with deuterium (9CI) (CA INDEX NAME)



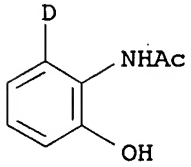

RN 98624-50-1 CAPLUS
CN Acetamide, N-(4-ethoxyphenyl-2,6-d2)- (9CI) (CA INDEX NAME)



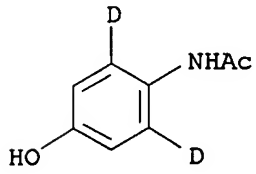

RN 98624-51-2 CAPLUS
CN Acetamide, N-(4-formylphenyl-2,6-d2)- (9CI) (CA INDEX NAME)



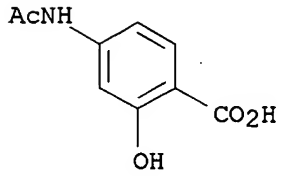

RN 98624-52-3 CAPLUS
CN Acetamide, N-(6-hydroxyphenyl-2-d)- (9CI) (CA INDEX NAME)



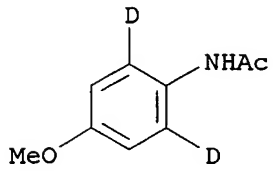

RN 98624-53-4 CAPLUS
CN Acetamide, N-(4-hydroxyphenyl-2,6-d2)- (9CI) (CA INDEX NAME)



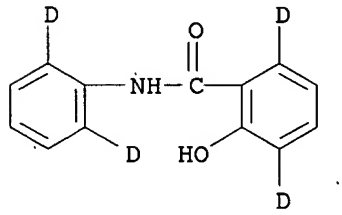
RN 98624-54-5 CAPLUS
CN Benzoic acid, 4-(acetylamino)-2-hydroxy-, labeled with deuterium (9CI) (CA INDEX NAME)



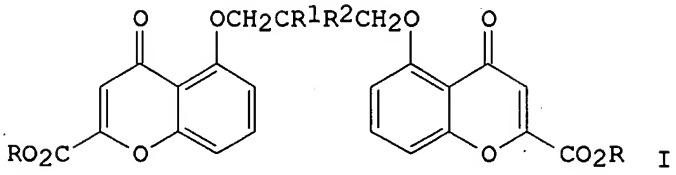

RN 98624-55-6 CAPLUS
CN Acetamide, N-(4-methoxyphenyl-2,6-d2)- (9CI) (CA INDEX NAME)




RN 98624-56-7 CAPLUS
CN Benzamide-2,5-d2, 6-hydroxy-N-(phenyl-2,6-d2)- (9CI) (CA INDEX NAME)




L24 ANSWER 63 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1984:591626 CAPLUS
DOCUMENT NUMBER: 101:191626
ORIGINAL REFERENCE NO.: 101:29030h,29031a
TITLE: Preparation of sodium cromoglycate (Intal) labeled with isotopic hydrogen
AUTHOR(S): Lockley, W. J. S.; Wilkinson, D. J.
CORPORATE SOURCE: Dep. Metab. Stud., Fisons PLC, Loughborough, LE11 0QY, UK
SOURCE: Journal of Labelled Compounds and Radiopharmaceuticals (1984), 21(4), 363-73
CODEN: JLCRD4; ISSN: 0362-4803
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 101:191626
GI



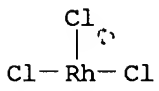
I

AB The title antiallergic drug I (R = Na, R1 = H, R2 = OH) (II) was labeled with D and T. II-6,6',8,8'-d4 was prepared by acid catalyzed exchange of cromoglycic acid with concentrated D2SO4 at 85° for 2 days and subsequent treatment with NaHCO3. The isotopomers I (R = Na, R1 = D, T, R2 = OH) were obtained from the oxo diacid I (R = H, R1R2 = O) by conversion to the Na salt I (R = Na, R1R2 = O) followed by reduction with NaBD4 and NaBT4, resp.; the tritiated isotopomer had a sp. activity of 1.99 Ci/mmol. II-3,3'-t2 was prepared with a sp. activity of 16.5 Ci/mmol by RhCl3-catalyzed exchange of cromoglycic acid with T2O at 90° for 24 h.

IT 10049-07-7
RL: CAT (Catalyst use); USES (Uses)
(catalysts, for exchange reaction of cromoglycic acid with tritium oxide)

RN 10049-07-7 CAPLUS

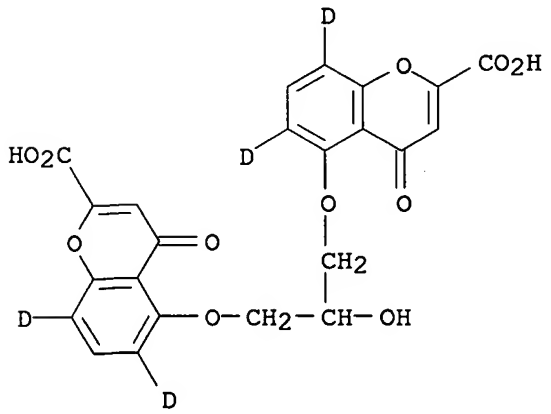
CN Rhodium chloride (RhCl3) (CA INDEX NAME)



IT 92588-97-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and conversion of, to sodium salt)

RN 92588-97-1 CAPLUS

CN 4H-1-Benzopyran-6,8-d2-2-carboxylic acid, 5,5'-[(2-hydroxy-1,3-propanediyl)bis(oxy)]bis[4-oxo- (9CI) (CA INDEX NAME)

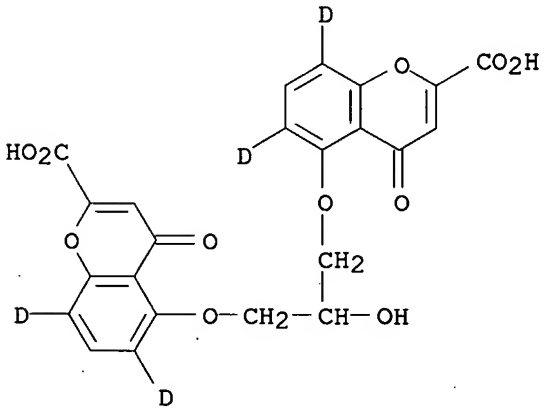


IT 92588-96-0P 92588-99-3P 92627-55-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 92588-96-0 CAPLUS

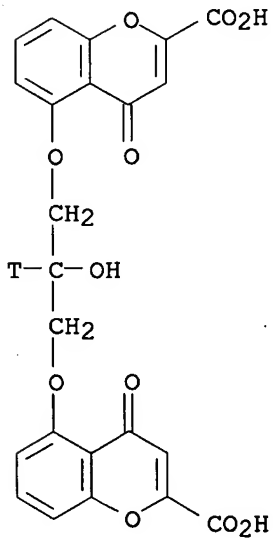
CN 4H-1-Benzopyran-6,8-d2-2-carboxylic acid, 5,5'-[(2-hydroxy-1,3-propanediyl)bis(oxy)]bis[4-oxo-, disodium salt (9CI) (CA INDEX NAME)



●2 Na

RN 92588-99-3 CAPLUS

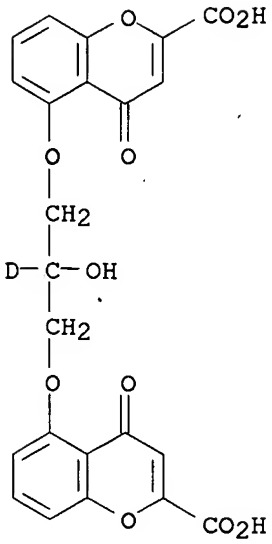
CN 4H-1-Benzopyran-2-carboxylic acid, 5,5'-[(2-hydroxy-1,3-propanediyl-2-t)bis(oxy)]bis[4-oxo-, disodium salt (9CI) (CA INDEX NAME)



●2 Na

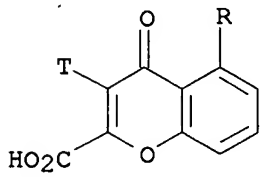
RN 92627-55-9 CAPLUS

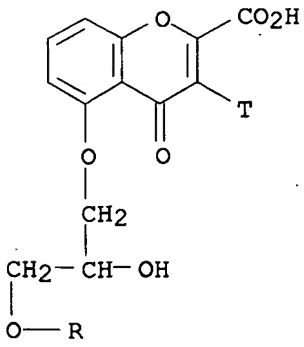
CN 4H-1-Benzopyran-2-carboxylic acid, 5,5'-[(2-hydroxy-1,3-propanediyl-2-d)bis(oxy)]bis[4-oxo-, disodium salt (9CI) (CA INDEX NAME)



●2 Na

IT 92588-95-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, ring cleavage, and decarboxylation of)
RN 92588-95-9 CAPLUS
CN 4H-1-Benzopyran-3-t-2-carboxylic acid, 5,5'-[(2-hydroxy-1,3-propanediyl)bis(oxy)]bis[4-oxo-, disodium salt (9CI) (CA INDEX NAME)





●2 Na

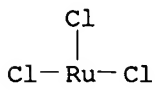
L24 ANSWER 64 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1984:530353 CAPLUS
DOCUMENT NUMBER: 101:130353
ORIGINAL REFERENCE NO.: 101:19821a,19824a

TITLE: Regioselective deuterium labeling of aromatic acids, amides, and amines using Group VIII metal catalysts
AUTHOR(S): Lockley, W. J. S.
CORPORATE SOURCE: Dep. Metab. Stud., Fisons PLC, Loughborough, LE11 0QY, UK
SOURCE: Journal of Labelled Compounds and Radiopharmaceuticals (1984), 21(1), 45-57
CODEN: JLCRD4; ISSN: 0362-4803
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 101:130353

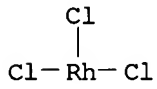
AB Aromatic carboxylic acids, amides, and amines were regioselectively ortho-deuterated by isotopic exchange with D2O in the presence of RhCl3.3H2O and other Group VIII metal complexes.

IT 10049-08-8 13569-65-8 15529-49-4
15825-24-8 71263-16-6
RL: CAT (Catalyst use); USES (Uses)
(catalysts, for regiospecific deuteration of aromatic carboxylic acids, amines, and amides)

RN 10049-08-8 CAPLUS
CN Ruthenium,chloride (RuCl3) (CA INDEX NAME)

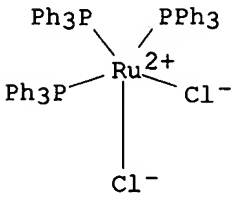


RN 13569-65-8 CAPLUS
CN Rhodium chloride (RhCl3), trihydrate (8CI, 9CI) (CA INDEX NAME)

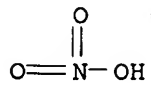


●3 $H_2O$

RN 15529-49-4 CAPLUS
CN Ruthenium, dichlorotris(triphenylphosphine)- (CA INDEX NAME)

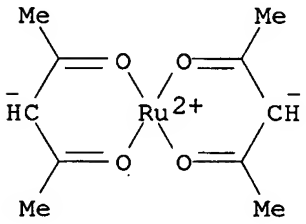


RN 15825-24-8 CAPLUS
CN Nitric acid, ruthenium(3+) salt (3:1) (CA INDEX NAME)

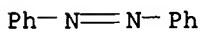


●1/3 Ru(III)

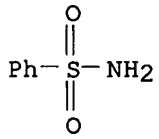
RN 71263-16-6 CAPLUS
CN Ruthenium, bis(2,4-pentanedionato-κO,κO')- (9CI) (CA INDEX NAME)



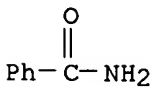
IT 91787-54-1P 91787-55-2P 91787-57-4P
91787-59-6P 91787-60-9P 91787-61-0P
91787-62-1P 91787-63-2P 91787-64-3P
91787-65-4P 91787-66-5P 91787-67-6P
91787-68-7P 91787-69-8P 91787-70-1P
937803-10-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by regiospecific, rhodium trichloride-catalyzed deuteration of arene)
RN 91787-54-1 CAPLUS
CN Diazene, diphenyl-, labeled with deuterium (9CI) (CA INDEX NAME)



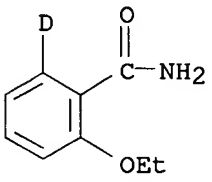
RN 91787-55-2 CAPLUS
CN Benzenesulfonamide, labeled with deuterium (9CI) (CA INDEX NAME)



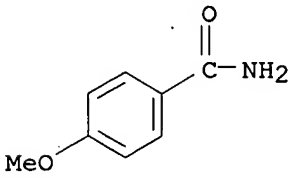
RN 91787-57-4 CAPLUS
CN Benzamide, labeled with deuterium (9CI) (CA INDEX NAME)



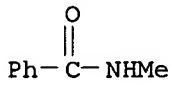
RN 91787-59-6 CAPLUS
CN Benzamide-2-d, 6-ethoxy- (9CI) (CA INDEX NAME)



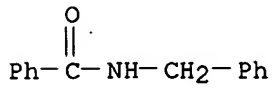
RN 91787-60-9 CAPLUS
CN Benzamide, 4-methoxy-, labeled with deuterium (9CI) (CA INDEX NAME)



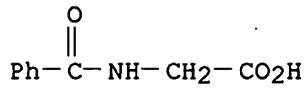
RN 91787-61-0 CAPLUS
CN Benzamide, N-methyl-, labeled with deuterium (9CI) (CA INDEX NAME)



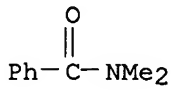
RN 91787-62-1 CAPLUS
CN Benzamide, N-(phenylmethyl)-, labeled with deuterium (9CI) (CA INDEX NAME)



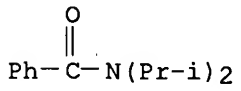
RN 91787-63-2 CAPLUS
CN Glycine, N-benzoyl-, labeled with deuterium (9CI) (CA INDEX NAME)



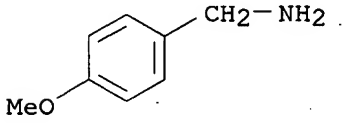
RN 91787-64-3 CAPLUS
CN Benzamide, N,N-dimethyl-, labeled with deuterium (9CI) (CA INDEX NAME)



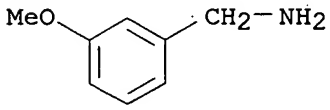
RN 91787-65-4 CAPLUS
CN Benzamide, N,N-bis(1-methylethyl)-, labeled with deuterium (9CI) (CA INDEX NAME)



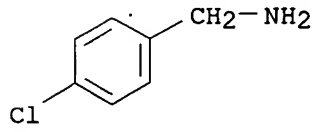
RN 91787-66-5 CAPLUS
CN Benzenemethanamine, 4-methoxy-, labeled with deuterium (9CI) (CA INDEX NAME)



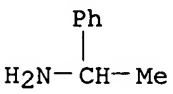
RN 91787-67-6 CAPLUS
CN Benzenemethanamine, 3-methoxy-, labeled with deuterium (9CI) (CA INDEX NAME)



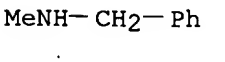
RN 91787-68-7 CAPLUS
CN Benzenemethanamine, 4-chloro-, labeled with deuterium (9CI) (CA INDEX NAME)



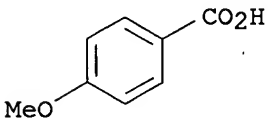
RN 91787-69-8 CAPLUS
CN Benzenemethanamine, α-methyl-, labeled with deuterium (9CI) (CA INDEX NAME)



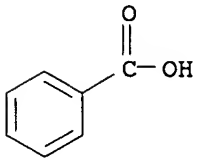
RN 91787-70-1 CAPLUS
CN Benzenemethanamine, N-methyl-, labeled with deuterium (9CI) (CA INDEX NAME)



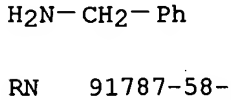
RN 937803-10-6 CAPLUS
CN Benzoic acid, 4-methoxy-, labeled with deuterium (CA INDEX NAME)



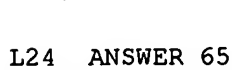
IT 85921-99-9P, preparation 91787-56-3P, preparation
91787-58-5P, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, regiospecific, rhodium trichloride-catalyzed deuteration of arene)
RN 85921-99-9 CAPLUS
CN Benzoic acid, labeled with deuterium (9CI) (CA INDEX NAME)



RN 91787-56-3 CAPLUS
CN Benzenemethanamine, labeled with deuterium (9CI) (CA INDEX NAME)

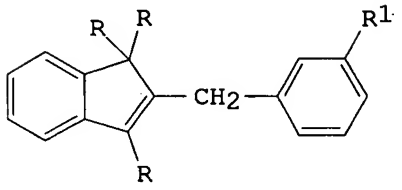


RN 91787-58-5 CAPLUS
CN Benzeneacetic acid, labeled with deuterium (9CI) (CA INDEX NAME)

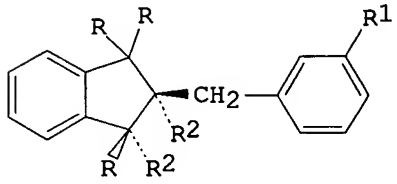


L24 ANSWER 65 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1984:490535 CAPLUS

DOCUMENT NUMBER: 101:90535
ORIGINAL REFERENCE NO.: 101:13871a,13874a
TITLE: Synthesis of regio- and stereospecifically deuterium labeled 2-benzylindans
AUTHOR(S): Kuch, Dietmar
CORPORATE SOURCE: Fak. Chem., Univ. Bielefeld, Bielefeld, D-4800, Fed. Rep. Ger.
SOURCE: Zeitschrift fuer Naturforschung, Teil B: Anorganische Chemie, Organische Chemie (1984), 39B(3), 369-74
CODEN: ZNBAD2; ISSN: 0340-5087
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

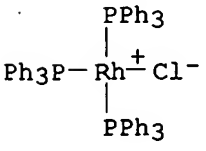



I



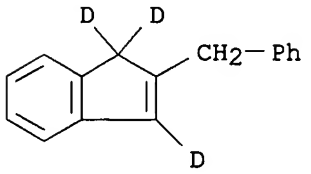

II

AB Treating benzylindenes I (R = H, R1 = H, OMe) with D2O, Et3N, and pyridine gave I (R = D, R1 = H, OMe). Hydrogenation of I (R = D, H; R1 = H, OMe) with H or D using ClRh(PPh3) as catalyst gave benzylindans II (R, R2 = H, D; R1 = H, OMe) with strict cis-1,2-addition of H/D to the double bond. Thus, stereo- and regiospecific D labeling occurred at the five-membered ring. The high selectivity of D incorporation was shown by 1H NMR and mass spectrometry.
IT 14694-95-2
RL: CAT (Catalyst use); USES (Uses)
(catalyst, for stereospecific deuteration of benzylindene)
RN 14694-95-2 CAPLUS
CN Rhodium, chlorotris(triphenylphosphine)-, (SP-4-2)- (CA INDEX NAME)

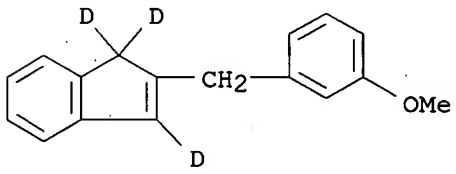



IT 91471-20-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrogenation of, stereochem. of)

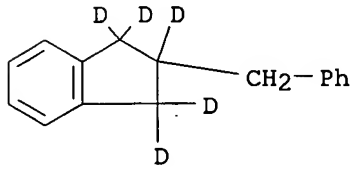
RN 91471-20-4 CAPLUS
CN 1H-Indene-1,1,3-d3, 2-(phenylmethyl)- (9CI) (CA INDEX NAME)



IT 91471-17-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrogenation of, stereochem. of)
RN 91471-17-9 CAPLUS
CN 1H-Indene-1,1,3-d3, 2-[(3-methoxyphenyl)methyl]- (9CI) (CA INDEX NAME)

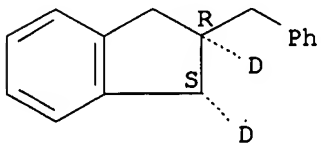


IT 77873-10-0P 77873-11-1P 77873-15-5P
91471-18-0P 91471-19-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 77873-10-0 CAPLUS
CN 1H-Indene-1,1,2,3-d4, 2,3-dihydro-3-d-2-(phenylmethyl)- (9CI) (CA INDEX NAME)



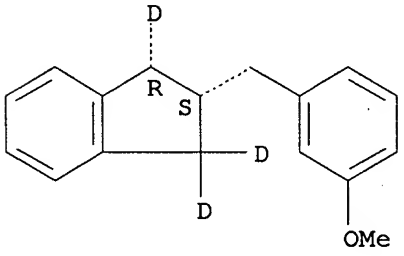
RN 77873-11-1 CAPLUS
CN 1H-Indene-1,2-d2, 2,3-dihydro-2-(phenylmethyl)-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



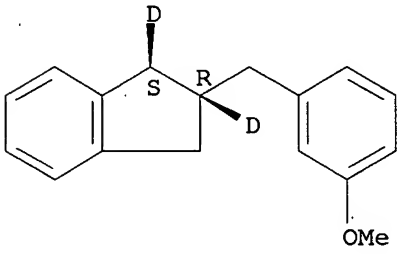
RN 77873-15-5 CAPLUS
CN 1H-Indene-1,1,3-d3, 2,3-dihydro-2-[(3-methoxyphenyl)methyl]-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



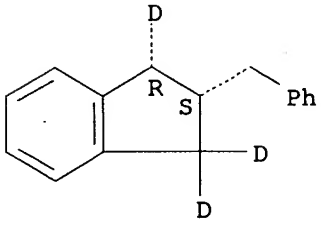

RN 91471-18-0 CAPLUS
CN 1H-Indene-1,2-d2, 2,3-dihydro-2-[(3-methoxyphenyl)methyl]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.




RN 91471-19-1 CAPLUS
CN 1H-Indene-1,1,3-d3, 2,3-dihydro-2-(phenylmethyl)-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



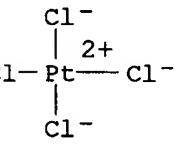

L24 ANSWER 66 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1984:407613 CAPLUS
DOCUMENT NUMBER: 101:7613
ORIGINAL REFERENCE NO.: 101:1311a,1314a
TITLE: Synthesis of deuterium and tritium labeled phenylglycine
AUTHOR(S): Kanska, M.

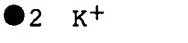
CORPORATE SOURCE: Dep. Chem., Univ. Warsaw, Warsaw, 02-093, Pol.
SOURCE: Journal of Radioanalytical and Nuclear Chemistry (1984), 85(4), 233-5
CODEN: JRNCDM; ISSN: 0236-5731
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The title labeled compds. were obtained by isotope exchange between phenylglycine and deuterated or tritiated water at elevated temperature in HCl medium using K2PtCl4 as a catalyst.

IT 10025-99-7
RL: CAT (Catalyst use); USES (Uses)
(catalysts, for deuteration of phenylglycine)

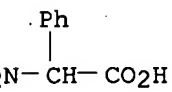
RN 10025-99-7 CAPLUS
CN Platinate(2-), tetrachloro-, potassium (1:2), (SP-4-1)- (CA INDEX NAME)



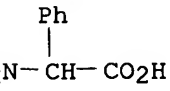


IT 90545-34-9P 90545-35-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 90545-34-9 CAPLUS
CN Benzeneacetic acid, α-amino-, labeled with deuterium (9CI) (CA INDEX NAME)

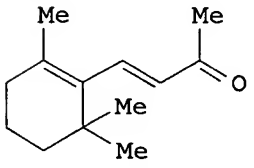


RN 90545-35-0 CAPLUS
CN Benzeneacetic acid, α-amino-, labeled with tritium (9CI) (CA INDEX NAME)



L24 ANSWER 67 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1983:4153 CAPLUS
DOCUMENT NUMBER: 98:4153
ORIGINAL REFERENCE NO.: 98:741a,744a
TITLE: Reduction of carbonyl compounds via hydrosilylation. 4. Highly regioselective reductions of α,β-unsaturated carbonyl compounds

AUTHOR(S): Ojima, Iwao; Kogure, Tetsuo
CORPORATE SOURCE: Sagami Chem. Res. Cent., Kanagawa, 229, Japan
SOURCE: Organometallics (1982), 1(10), 1390-9
CODEN: ORGND7; ISSN: 0276-7333
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

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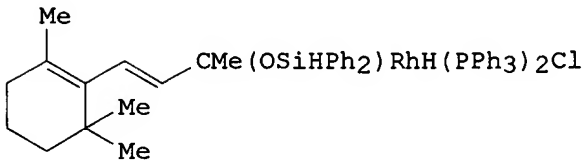
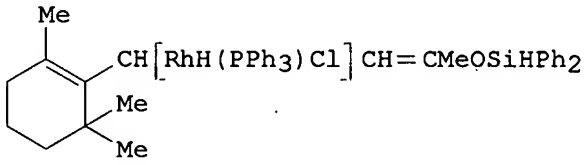
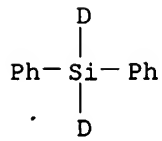



II




III

AB The highly regioselective reduction of α,β-unsatd. CO compds., to give the corresponding α,β-saturated CO compound (via 1,4--addition) or allylic alcs. (via 1,2-addition), was effected by ClRh(PPh3)3 catalyzed hydrosilylation followed by methanolysis of the resulting adducts. Regiospecific deuteration occurred when deuteriosilanes were used. The regioselectivity in the hydrosilylation depends on the type of hydrosilanes used; monohydrosilanes give silyl enol ethers (1,4-adduct) and dihydrosilanes give silyl ethers (1,2-adduct). Other regioselectivity controlling factors are the CO compound structure, the hydrosilane-substrate ratio, solvent, and the reaction temperature Spin trapping of radical intermediates in the reaction of Ph2SiH2 with I (the ESR of the adducts are assigned), by 2,3,5,6-Me4C6HNO, support the intermediacy of II and III for the 1,2- and 1,4-addition reactions, resp. The factors which affect the interconversion of II and III, the H- shift in their decomposition, and the catalysis of this step by silanes are discussed.
IT 17950-94-6
RL: PRP (Properties)
(deuteriogeranial from)
RN 17950-94-6 CAPLUS
CN Silane-d2, diphenyl- (CA INDEX NAME)

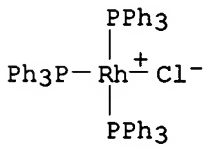



IT 14694-95-2
RL: CAT (Catalyst use); USES (Uses)

(hydrosilylation catalyst, for α,β-unsatd. carbonyl compds., mechanism and regioselectivity with)

RN 14694-95-2 CAPLUS

CN Rhodium, chlorotris(triphenylphosphine)-, (SP-4-2)- (CA INDEX NAME)



IT 82798-39-8P

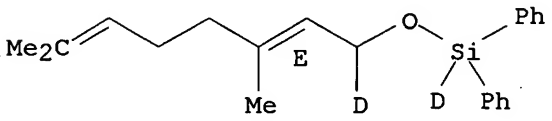
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and methanolysis of)

RN 82798-39-8 CAPLUS

CN Silane-d, [(3,7-dimethyl-2,6-octadienyl-1-d)oxy]diphenyl-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L24 ANSWER 68 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1982:181453 CAPLUS

DOCUMENT NUMBER: 96:181453

ORIGINAL REFERENCE NO.: 96:29907a,29910a

TITLE: Triterpenes. LXV. Homogeneous hydrogenation and deuteration of pentacyclic triterpenoids: double bonds in side chains

AUTHOR(S): Protiva, Jiri; Lepsa, Ludek; Klinotova, Eva; Klinot, Jiri; Krecek, Vaclav; Vystrcil, Alois

CORPORATE SOURCE: Dep. Org. Chem., Charles Univ., 128 40, Czech.

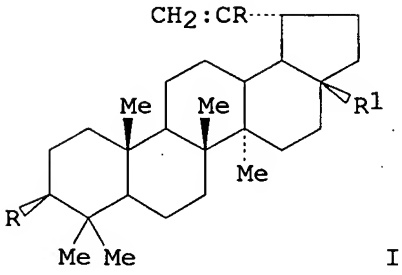
SOURCE: Collection of Czechoslovak Chemical Communications (1981), 46(11), 2734-41

CODEN: CCCCAK; ISSN: 0366-547X

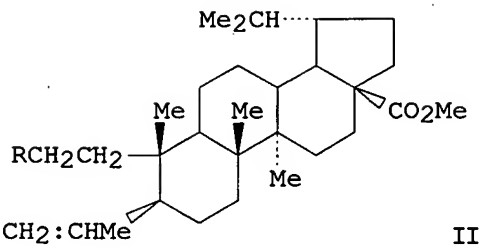
DOCUMENT TYPE: Journal

LANGUAGE: English

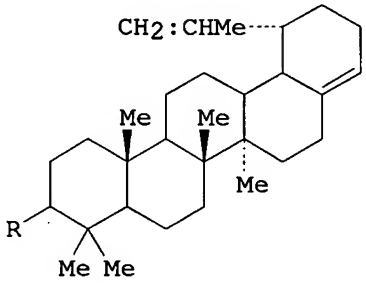
GI




I




II



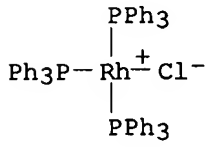

III

AB Reaction conditions, such as type of solvent, reaction time, and amount of catalyst, were studied in the (Ph3P)3RhCl-catalyzed hydrogenation and deuteration of double bonds in 29 terpenoids (I-III). Both isolated and conjugated dienes were hydrogenated, whereas the cyano group was stable. Selective hydrogenation of mono- or disubstituted terminal double bonds depended on the solvent polarity. Regioselectivity of D over the mol. after deuteration was solvent dependent, too.

IT 14694-95-2
RL: CAT (Catalyst use); USES (Uses)
(catalysts, for deuteration and hydrogenation of lupenes and norlupenes)

RN 14694-95-2 CAPLUS

CN Rhodium, chlorotris(triphenylphosphine)-, (SP-4-2)- (CA INDEX NAME)

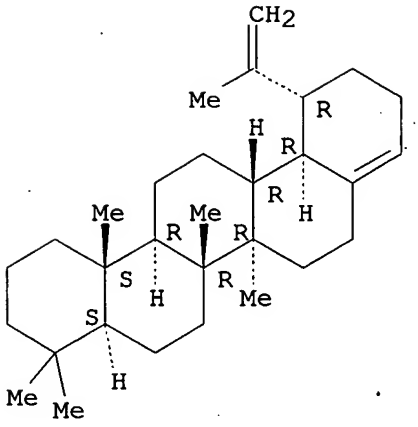



IT 81345-99-5P 81346-00-1P 81346-01-2P
81362-22-3P 81362-23-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by deuteration of lupene or norlupene derivative)

RN 81345-99-5 CAPLUS

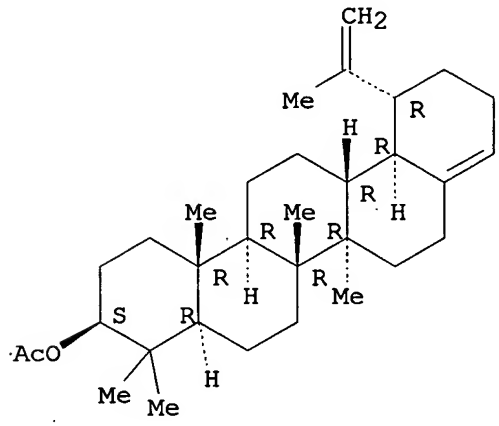
CN 28,29,30-Trinorgammacer-17(22)-ene, 19-(1-methylethenyl)-, labeled with deuterium, (19α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



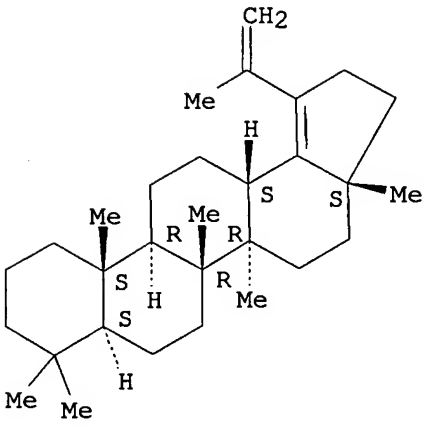
RN 81346-00-1 CAPLUS
CN 28,29,30-Trinorgammacer-17(22)-en-3-ol, 19-(1-methylethenyl)-, acetate, labeled with deuterium, (3β,19α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



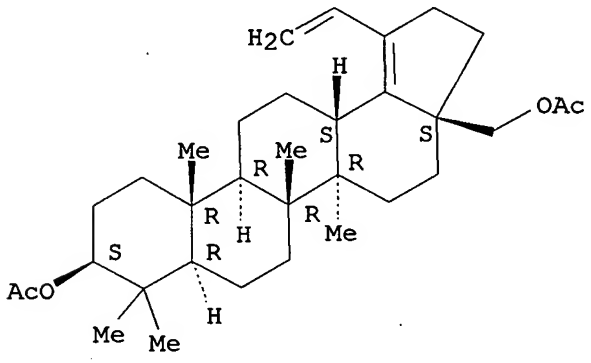
RN 81346-01-2 CAPLUS
CN Lupa-18,20(29)-diene, labeled with deuterium (9CI) (CA INDEX NAME)

Absolute stereochemistry.



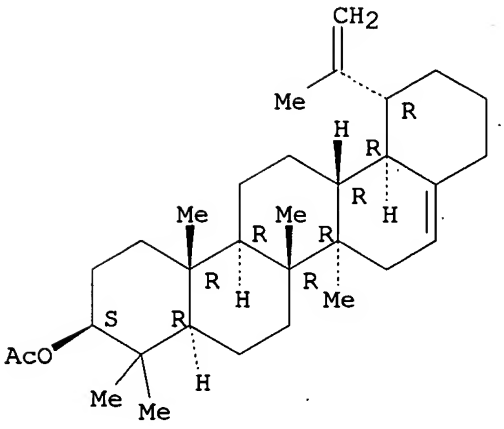
RN 81362-22-3 CAPLUS
CN 30-Norlupa-18,20(29)-diene-3,28-diol, diacetate, labeled with deuterium, (3β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 81362-23-4 CAPLUS
CN E-Homolupa-16,20(29)-dien-3-ol, acetate, labeled with deuterium, (3β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



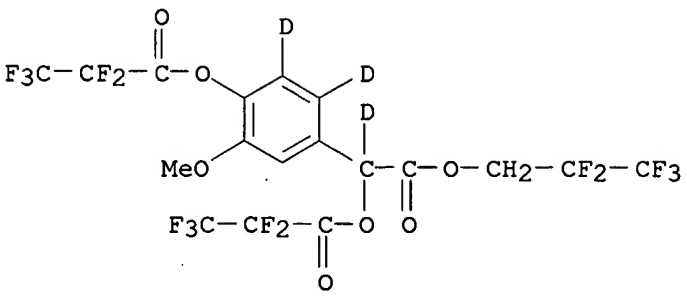
L24 ANSWER 69 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1982:34752 CAPLUS
DOCUMENT NUMBER: 96:34752
ORIGINAL REFERENCE NO.: 96:5737a,5740a
TITLE: Deuterated biogenic amine metabolites: preparation of ring-deuterated 4-hydroxy-3-methoxymandelic acid
AUTHOR(S): Faull, Kym F.; Anderson, Patricia J.; Barchas, Jack D.
CORPORATE SOURCE: Dep. Psychiatry Behav. Sci., Stanford Univ. Sch. Med., Stanford, CA, 94305, USA
SOURCE: Journal of Labelled Compounds and Radiopharmaceuticals (1981), 18(7), 1075-9
CODEN: JLCRD4; ISSN: 0362-4803
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Ring deuterated derivs. of the title compound were prepared by Pt-catalyzed exchange reaction with D2O (sealed, degassed ampul, room temperature, 3 wk). Under these conditions, the trideuterated derivative was the major product (70%). The pentafluoropropionyl derivative of the product was prepared and its mass spectrum was resolved.

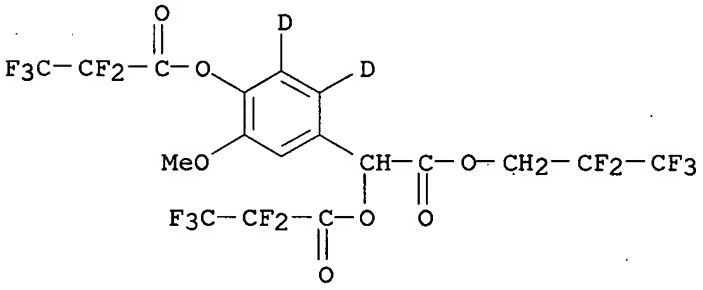
IT 7440-06-4, uses and miscellaneous
RL: CAT (Catalyst use); USES (Uses)
(catalysts, for regioselective deuteration of hydroxymethoxymandelic acid)
RN 7440-06-4 CAPLUS
CN Platinum (CA INDEX NAME)

Pt

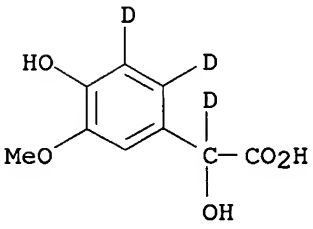
IT 80333-83-1P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and mass spectrum of)
RN 80333-83-1 CAPLUS
CN Benzene-2,3-d2-acetic-α-d acid, 5-methoxy-α,4-bis(2,2,3,3,3-pentafluoro-1-oxopropoxy)-, 2,2,3,3,3-pentafluoropropyl ester (9CI) (CA INDEX NAME)



IT 80333-84-2P 80333-85-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 80333-84-2 CAPLUS
CN Benzene-2,3-d2-acetic acid, 5-methoxy-α,4-bis(2,2,3,3,3-pentafluoro-1-oxopropoxy)-, 2,2,3,3,3-pentafluoropropyl ester (9CI) (CA INDEX NAME)



RN 80333-85-3 CAPLUS
CN Benzene-2,3-d2-acetic-α-d acid, α,4-dihydroxy-5-methoxy- (9CI) (CA INDEX NAME)



L24 ANSWER 70 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1980:639868 CAPLUS
DOCUMENT NUMBER: 93:239868
ORIGINAL REFERENCE NO.: 93:38447a,38450a
TITLE: Synthesis of deuterium and tritium labelled tyrosine
AUTHOR(S): Kanska, M.; Drabarek, S.
CORPORATE SOURCE: Inst. Fundam. Probl. Chem., Warsaw Univ., Warsaw, 02-093, Pol.
SOURCE: Radiochemical and Radioanalytical Letters (1980),

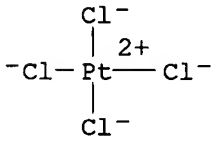
44(4), 207-10
CODEN: RRALAZ; ISSN: 0079-9483
DOCUMENT TYPE: Journal
LANGUAGE: English

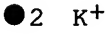
AB Tyrosine was deuterated and tritiated in the aromatic ring by isotope exchange reactions in D2O or HTO containing HCl at 100° by catalysis with K2PtCl4. The deuteration at 100° for 69 h gave full deuterium substitution in positions 3 and 5, but only 50% deuteration in positions 2 and 6.

IT 10025-99-7
RL: CAT (Catalyst use); USES (Uses)
(catalysts, for deuteration and tritiation of tyrosine)

RN 10025-99-7 CAPLUS

CN Platinate(2-), tetrachloro-, potassium (1:2), (SP-4-1)- (CA INDEX NAME)



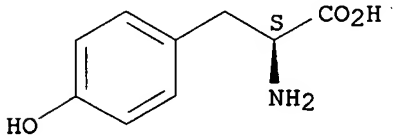


IT 61911-91-9P, preparation 75684-54-7P, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 61911-91-9 CAPLUS

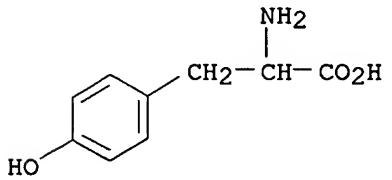
CN L-Tyrosine, labeled with deuterium (9CI) (CA INDEX NAME)

Absolute stereochemistry.



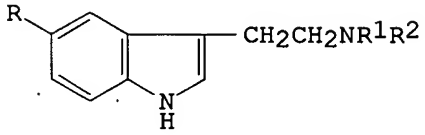
RN 75684-54-7 CAPLUS

CN L-Tyrosine, labeled with tritium (9CI) (CA INDEX NAME)



L24 ANSWER 71 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1979:405443 CAPLUS
DOCUMENT NUMBER: 91:5443

ORIGINAL REFERENCE NO.: 91:1022h,1023a
TITLE: Deuterium labeling of tryptamine, serotonin and their N-methylated metabolites using solvent exchange reactions
AUTHOR(S): Raisanen, Martti; Karkkainen, Jorma
CORPORATE SOURCE: Dep. Med. Chem., Univ. Helsinki, Helsinki, SF-00170/17, Finland
SOURCE: Acta Chemica Scandinavica, Series B: Organic Chemistry and Biochemistry (1979), B33(1), 11-14
CODEN: ACBOCV; ISSN: 0302-4369
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



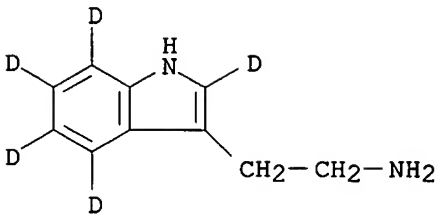

I

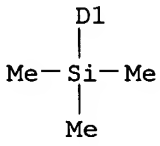
AB Tryptamine (I, R - R2 = H), serotonin (I, R = OH, R1 = R2 = H), and their N-methylated metabolites I (R = H, OH, R1 = H, Me, R2 = Me) were deuterated by the title method with heterogeneous Pt-catalysis in 30% AcOD-D2O or by homogeneous acid catalysis with 2M D2SO4 in D2O. The deuterated trimethylsilyl derivs. were characterized by their mass spectra. The deuteriums were attached to the indole nucleus.

IT 7440-06-4, uses and miscellaneous
RL: CAT (Catalyst use); USES (Uses)
(catalysts, for deuteration of tryptamine and serotonin and their N-methylated metabolites by solvent exchange reactions)
RN 7440-06-4 CAPLUS
CN Platinum (CA INDEX NAME)

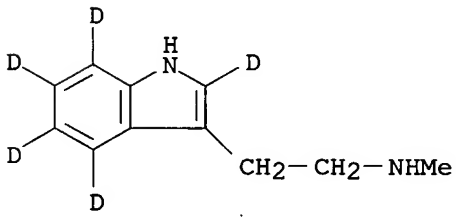
Pt

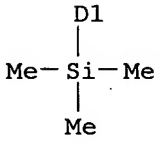
IT 70455-42-4 70455-43-5 70455-44-6
70455-45-7 70455-46-8 70463-09-1
RL: PRP (Properties)
(mass spectrum of)
RN 70455-42-4 CAPLUS
CN 1H-Indole-2,4,5,6,7-d5-3-ethanamine, N(or 1)-(trimethylsilyl)- (9CI) (CA INDEX NAME)



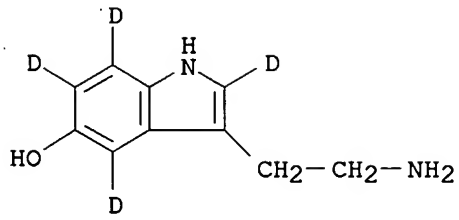


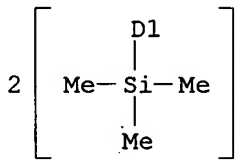
RN 70455-43-5 CAPLUS
CN 1H-Indole-2,4,5,6,7-d5-3-ethanamine, N-methyl-N(or 1)-(trimethylsilyl)-(9CI) (CA INDEX NAME)



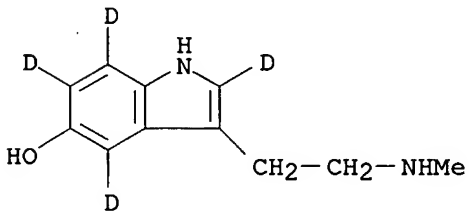


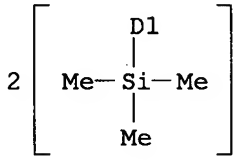
RN 70455-44-6 CAPLUS
CN 1H-Indol-2,4,6,7-d4-5-ol, 3-(2-aminoethyl)-, bis(trimethylsilyl) deriv. (9CI) (CA INDEX NAME)



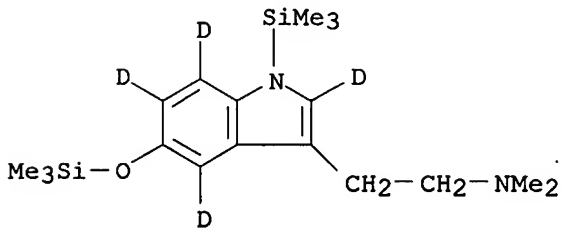


RN 70455-45-7 CAPLUS
CN 1H-Indol-2,4,6,7-d4-5-ol, 3-[2-(methylamino)ethyl]-, bis(trimethylsilyl) deriv. (9CI) (CA INDEX NAME)



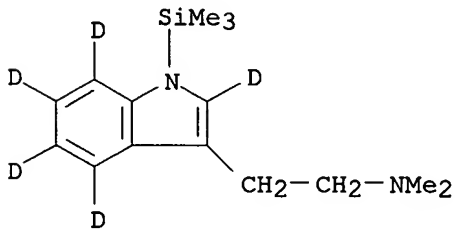


RN 70455-46-8 CAPLUS
CN 1H-Indole-2,4,8,7-d4-3-ethanamine, N,N-dimethyl-1-(trimethylsilyl)-5-[(trimethylsilyl)oxy]- (9CI) (CA INDEX NAME)



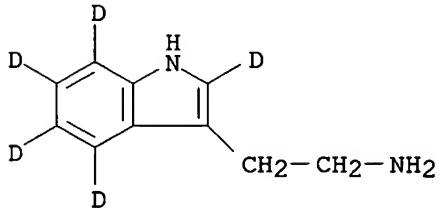
RN 70463-09-1 CAPLUS

CN 1H-Indole-2,4,5,6,7-d5-3-ethanamine, N,N-dimethyl-1-(trimethylsilyl)- (9CI) (CA INDEX NAME)

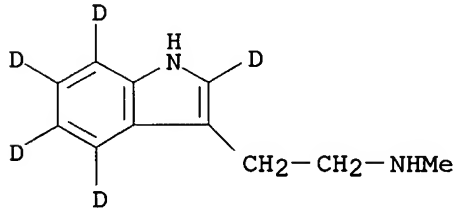


IT 70463-03-5P 70463-04-6P 70463-05-7P
70463-06-8P 70463-07-9P 70463-08-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by deuteration by acid- or platinum-catalyzed solvent exchange reaction)

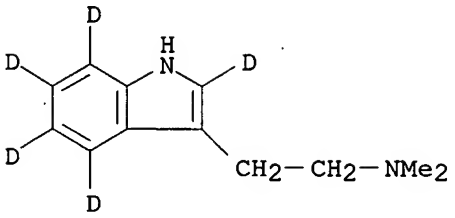
RN 70463-03-5 CAPLUS
CN 1H-Indole-2,4,5,6,7-d5-3-ethanamine (9CI) (CA INDEX NAME)



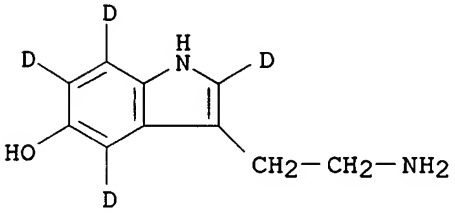
RN 70463-04-6 CAPLUS
CN 1H-Indole-2,4,5,6,7-d5-3-ethanamine, N-methyl- (9CI) (CA INDEX NAME)



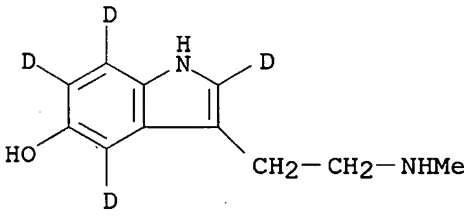
RN 70463-05-7 CAPLUS
CN 1H-Indole-2,4,5,6,7-d5-3-ethanamine, N,N-dimethyl- (9CI) (CA INDEX NAME)



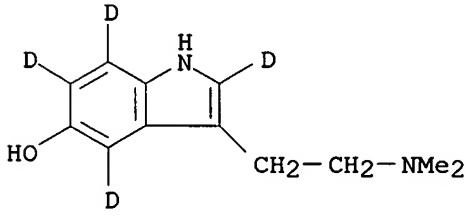
RN 70463-06-8 CAPLUS
CN 1H-Indol-2,4,6,7-d4-5-ol, 3-(2-aminoethyl)- (9CI) (CA INDEX NAME)



RN 70463-07-9 CAPLUS
CN 1H-Indol-2,4,6,7-d4-5-ol, 3-[2-(methylamino)ethyl]- (9CI) (CA INDEX NAME)



RN 70463-08-0 CAPLUS
CN 1H-Indol-2,4,6,7-d4-5-ol, 3-[2-(dimethylamino)ethyl]- (9CI) (CA INDEX NAME)

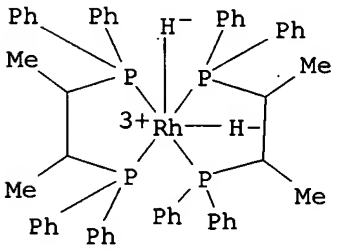


L24 ANSWER 72 OF 72 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1977:602062 CAPLUS
DOCUMENT NUMBER: 87:202062

ORIGINAL REFERENCE NO.: 87:32011a,32014a
TITLE: Asymmetric synthesis. Production of optically active amino acids by catalytic hydrogenation
AUTHOR(S): Fryzuk, M. D.; Bosnich, B.
CORPORATE SOURCE: Chem. Dep., Univ. Toronto, Toronto, ON, Can.
SOURCE: Journal of the American Chemical Society (1977), 99(19), 6262-7
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English

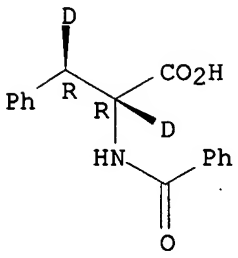
AB RCH:C(NHR1)CO2H [R = H, Ph, Me2CH, p-(HO)C6H4, p-(AcO)C6H4, 3,4-(MeO)(AcO)C6H3; R1 = Ac, Bz] underwent asym. hydrogenation over [Rh[(S,S)-chiraphos](NBD)]ClO4 [I; (S,S)-chiraphos = (2S,3S)-MeCH(PPh2)CH(PPh2)Me, NBD = norbornadiene] in THF, EtOH, benzene, or dioxane to give the appropriate acylated R-amino acid with optical yields of 72-100%. [Rh[(S,S)-chiraphos)(H)2(solvent)2]+ is the species which hydrogenates the olefin under catalytic conditions. (2R,3R)-MeCH(OTos)CH(OTos)Me (Tos = tosyl) was treated with LiPPh2, Ni(ClO4)2, and NaSCN to give a Ni complex which was treated with NaCN to give (S,S)-chiraphos which was treated with [Rh(NBD)(AcAc)] and HClO4 to give I. I was also used to catalyze the asym. deuteration of BzNHCH:CHCO2H.

IT 65013-93-6
RL: CAT (Catalyst use); USES (Uses)
(catalyst, for asym. hydrogenation of acylaminoacrylic acids)
RN 65013-93-6 CAPLUS
CN Rhodium(1+), bis[(1,2-dimethyl-1,2-ethanediyl)bis[diphenylphosphine]-P,P']dihydro- (9CI) (CA INDEX NAME)




IT 64896-29-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and racemization of)
RN 64896-29-3 CAPLUS
CN D-Phenylalanine-α,β-d2, N-benzoyl-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.




=>

---Logging off of STN---

=>
Executing the logoff script...

=> LOG Y

| COST IN U.S. DOLLARS | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| FULL ESTIMATED COST | 394.32 | 932.01 |

| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE ENTRY | TOTAL SESSION |
|---|---|---|
| CA SUBSCRIBER PRICE | -57.60 | -59.95 |

STN INTERNATIONAL LOGOFF AT 10:28:12 ON 16 JUL 2008